Supporting Information

High H_2 uptake in pure, Li-, Na-, K-metalated Covalent Organic Frameworks and Metal Organic Frameworks at 298 K

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1 Comparison of CCSD, M06 and B3LYP for the Li-Li binding energy

For the case of Li-Li binding energy, UDFT/MO6/6-311G**++ gives a similar profile to the CCSD results. Li-Li energy with respect to the coordinate distance in Fig. S1 shows that the UDFT/B3LYP/6-311G**++ gives the worst results for this case. J.L.M.-C. would like to thank Wei-Guang Liu for providing this CCSD curve.

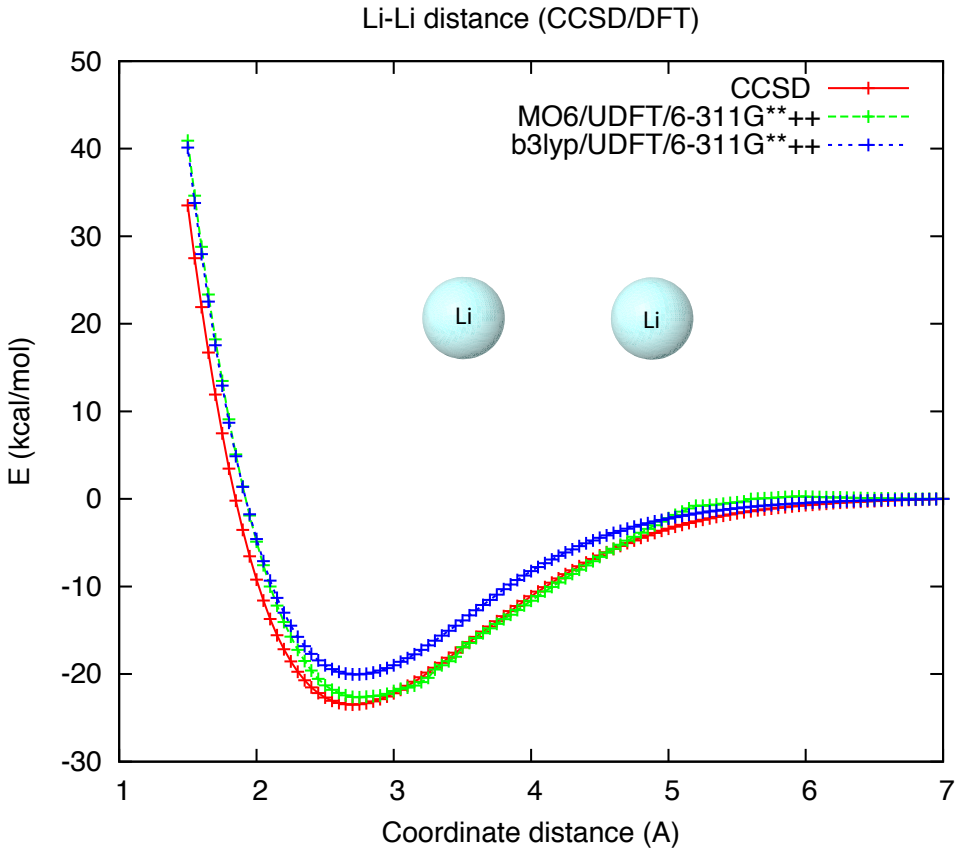


Figure S1: Li-Li binding energy

2 Formulation

2.1 Excess absorption

In sorption experiments, the excess amount is obtained but the absolute amount can only be estimated. The absolute adsorbed amount can be estimated from experimental data by using[1],

$$N_{\text{total}} = N_{\text{excess}} + V_{\text{p}} \times \rho_{\text{bulk}} \tag{1}$$

where N_{excess} is the excess mass, V_{p} is the pore volume, N_{total} is the total adsorbed amount of H_2 and ρ_{bulk} is the bulk density of H_2. However from our GCMC calculations we obtain N_{total} directly.

2.2 Effective absorption

A second definition to estimate the amount of H_2 absorbed is by the concept of effective adsorption uptake, $N_{\text{effective}}$ has the following formulation [2]:

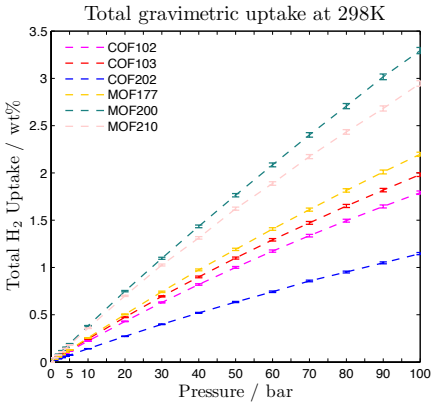
$$N_{\text{total}} = N_{\text{effective}} + V_{\text{cell}} \times \rho_{\text{bulk}} \tag{2}$$

where $N_{\text{effective}}$ is the affective mass of hydrogen uptake absorbed, V_{cell} is the volume of the cell occupied by the framework, N_{total} is total adsorbed amount of H_2 and ρ_{bulk} is the bulk density of H_2. Again from our GCMC we obtain N_{total} directly.

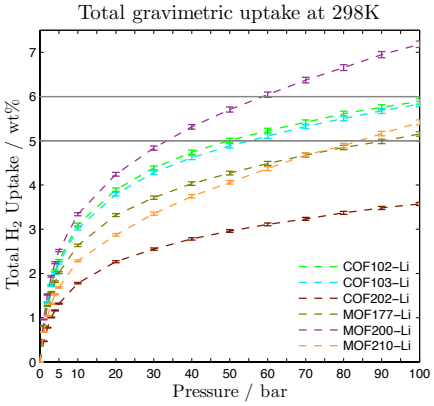
The *excess* amount quantity only takes into account the free pore volume and this does not capture the phenomena of ratio of size of framework to their storage capacity, while the *effective* unit takes into account the size of the framework and the alkaline metal in a more proper way.

3 Gravimetric uptake

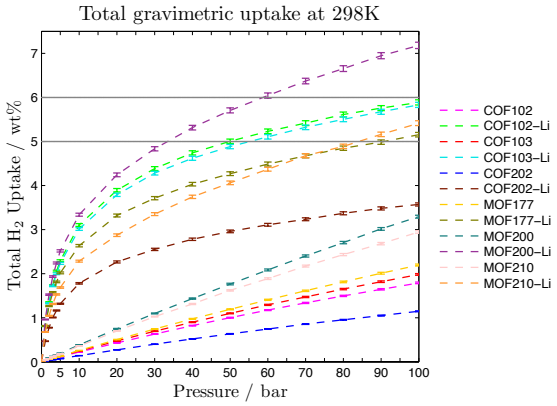
3.1 Total gravimetric uptake (wt%)



2.1: Unmetalated wt% total

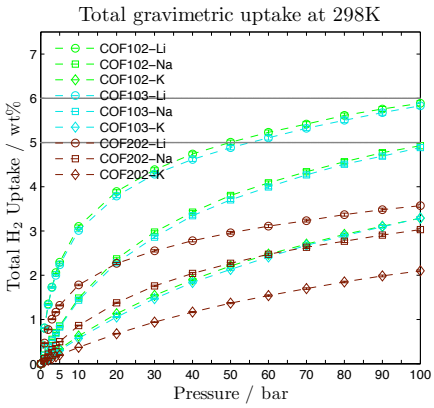


2.2: Li-metalated wt% total

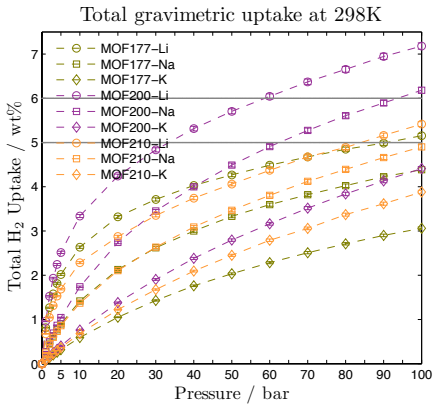


2.3: All wt% total

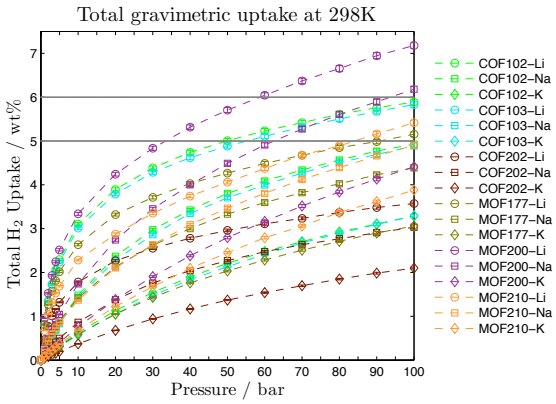
Figure S2: wt% total of metalated and Li-metalated frameworks (note the changes in the y-axis scale)



3.1: All metalated COFs

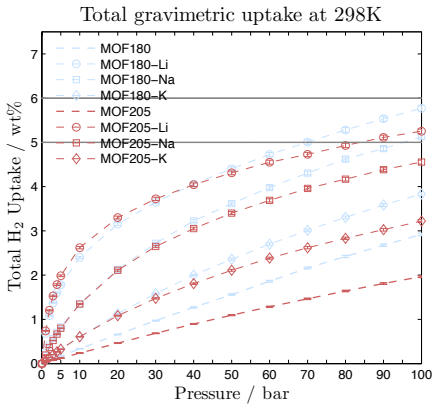


3.2: All metalated MOFs



3.3: All metalated wt% tot.

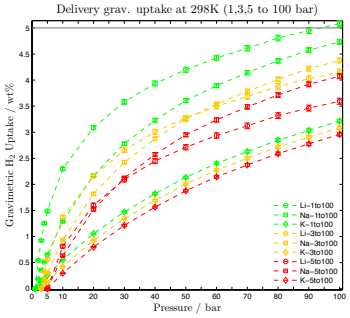
Figure S3: wt% total of Li-,Na-,K-metalated frameworks



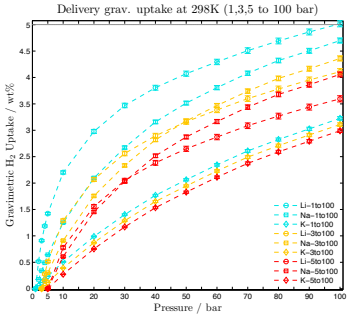
4.1: MOF180 and MOF205

Figure S4: Wt% total of Li-,Na-,K-metalated and unmetalated MOF180 and MOF205

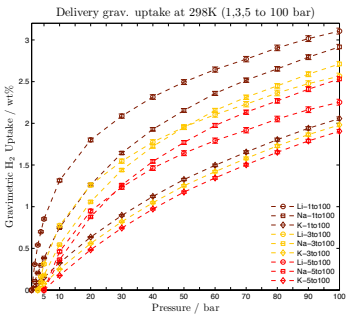
3.2 Delivery gravimetric uptake (wt% delivery)



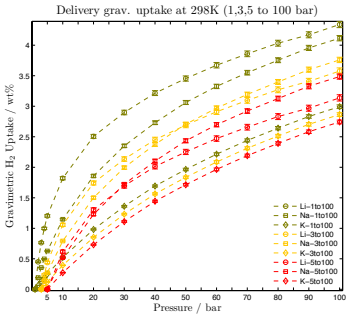
5.1: COF102 wt% delivery



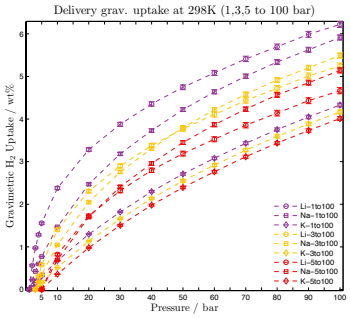
5.2: COF103 wt% delivery



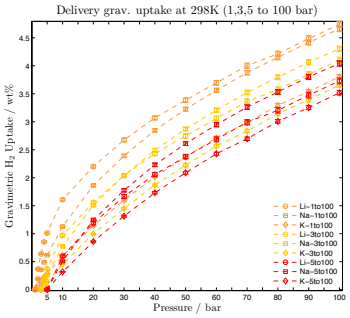
5.3: COF202 wt% delivery



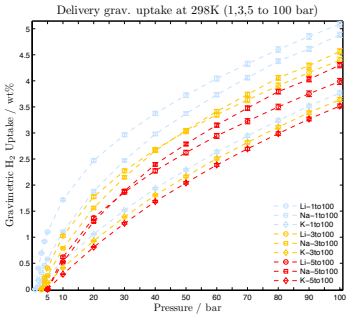
5.4: MOF177 wt% delivery



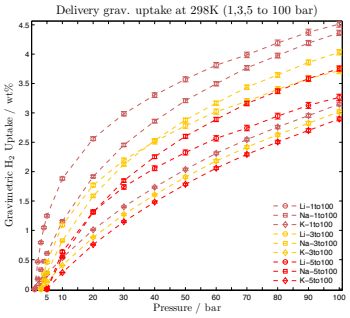
5.5: MOF200 wt% delivery



5.6: MOF210 wt% delivery

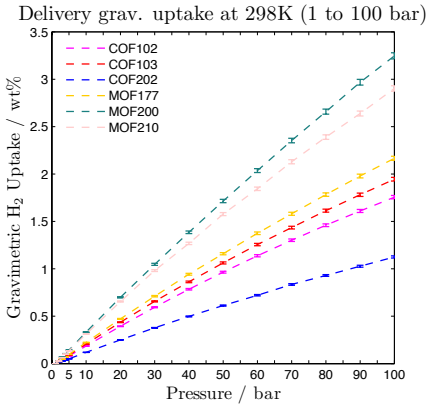


5.7: MOF180 wt% delivery

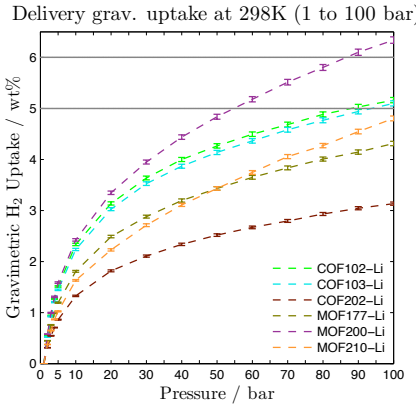


5.8: MOF205 wt% delivery

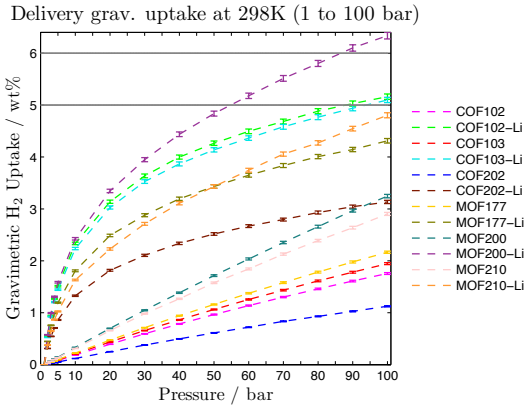
Figure S5: Wt% delivery of Li-,Na-,K-metalated frameworks at different references (1 to 100 bar, 3 to 100 bar & 5 to 100 bar) (note the changes in the y-axis scale)



6.1: Unmetalated wt% delivery (1 to 100 bar)

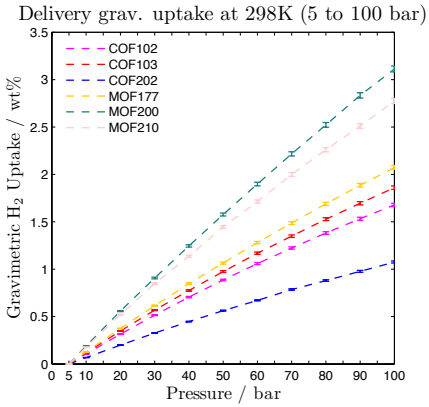


6.2: Li-metalated wt% delivery (1 to 100 bar)

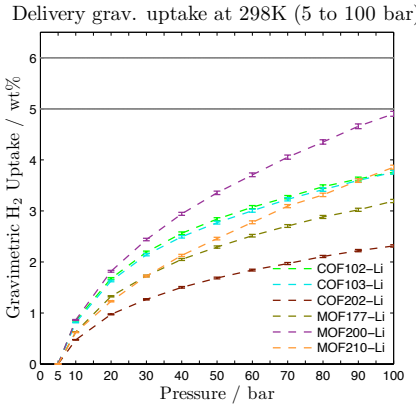


6.3: All wt% delivery (1 to 100 bar)

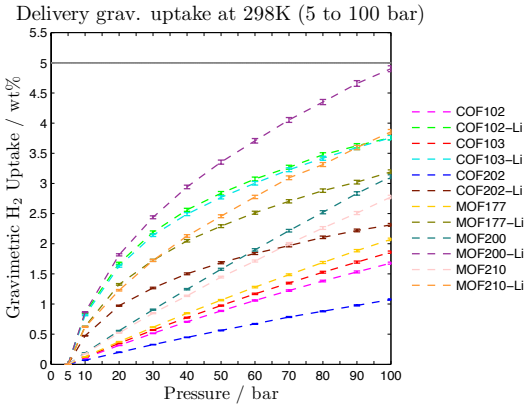
Figure S6: Wt% delivery of unmetalated and Li-metalated frameworks (note the changes in the y-axis scale). The reference is 1 bar.



7.1: Unmetalated wt% delivery (5 to 100 bar)

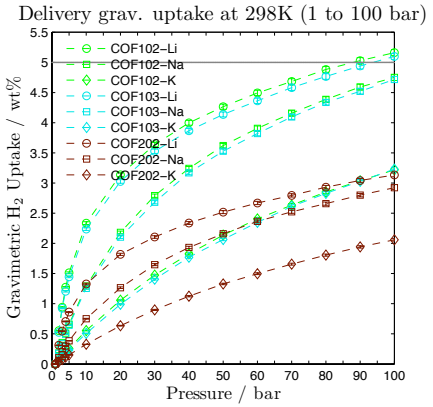


7.2: Li-metalated wt% delivery (5 to 100 bar)

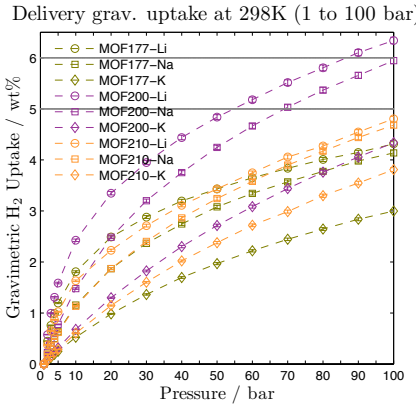


7.3: All wt% delivery (5 to 100 bar)

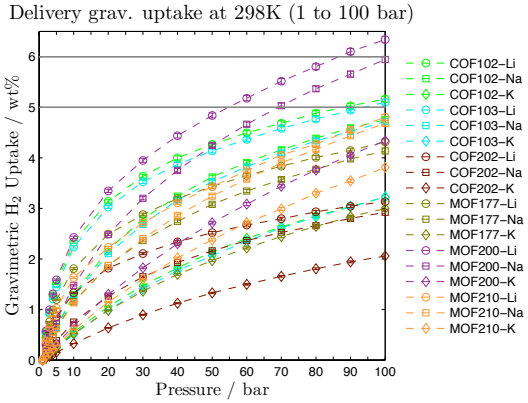
Figure S7: Wt% delivery of unmetalated and Li-metalated frameworks (note the changes in the y-axis scale). The reference is 5 bar.



8.1: All metalated COFs (1 to 100 bar)

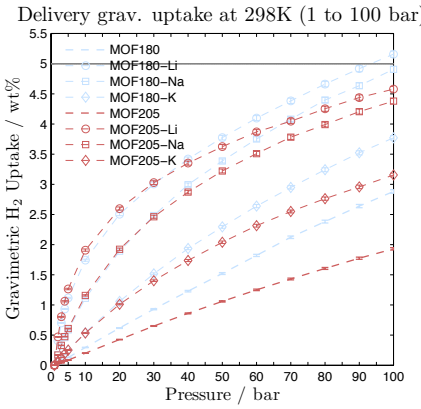


8.2: All metalated MOFs (1 to 100 bar)



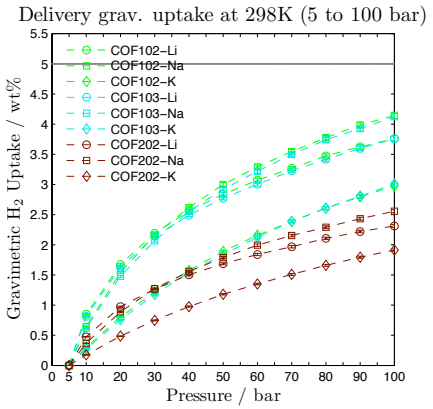
8.3: All metalated wt% delivery (1 to 100 bar)

Figure S8: wt% delivery of Li-,Na-,K-metalated frameworks. The reference is 1 bar.

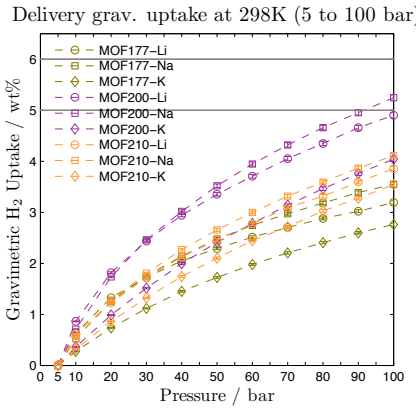


9.1: MOF180 and MOF205 (1 to 100 bar)

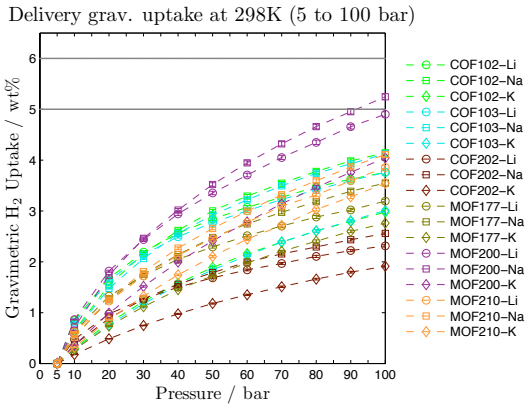
Figure S9: Wt% delivery of Li-,Na-,K-metalated and unmetalated MOF180 and MOF205. The reference is 1 bar.



10.1: All metalated COFs (5 to 100 bar)

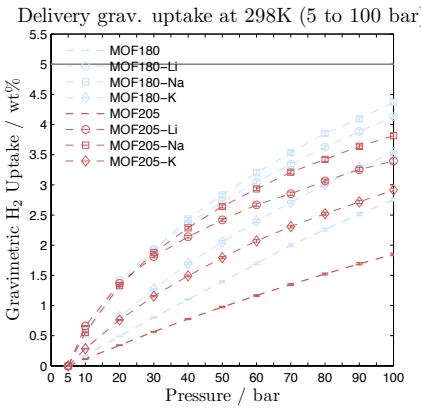


10.2: All metalated MOFs (5 to 100 bar)



10.3: All metalated wt% delivery (5 to 100 bar)

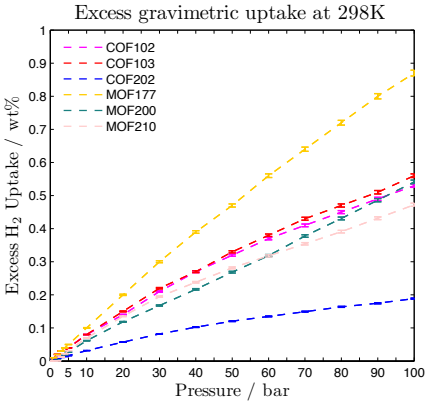
Figure S10: wt% delivery of Li-,Na-,K-metalated frameworks. The reference is 5 bar.



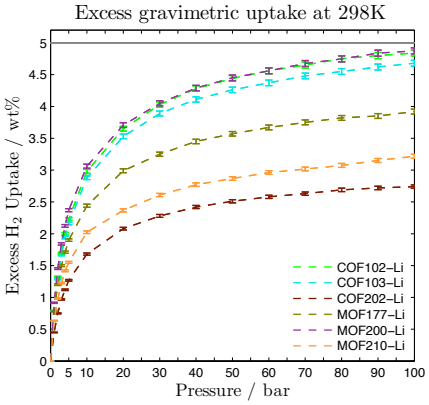
11.1: MOF180 and MOF205 (5 to 100 bar)

Figure S11: Wt% delivery of Li-,Na-,K-metalated and unmetalated MOF180 and MOF205. The reference is 5 bar.

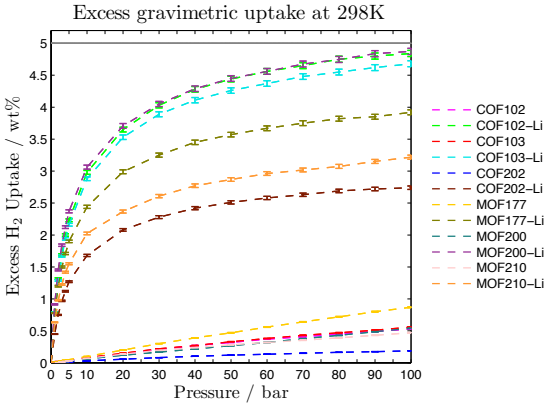
3.3 Excess gravimetric uptake (wt% excess)



12.1: Unmetalated wt% excess

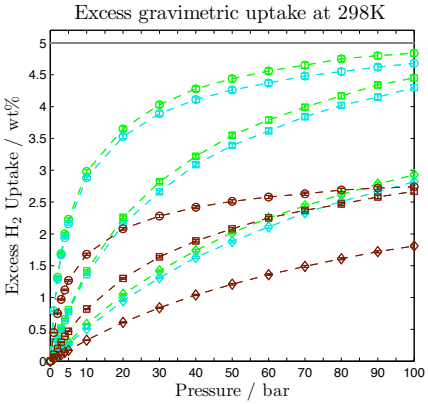


12.2: Li-metalated wt% excess

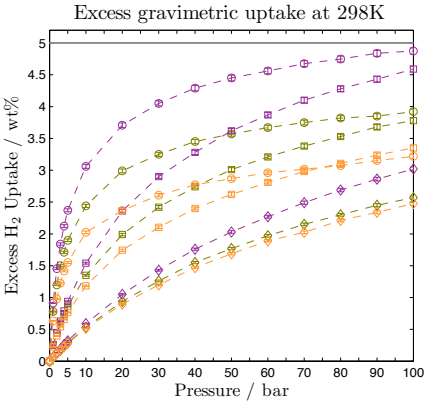


12.3: All wt% excess

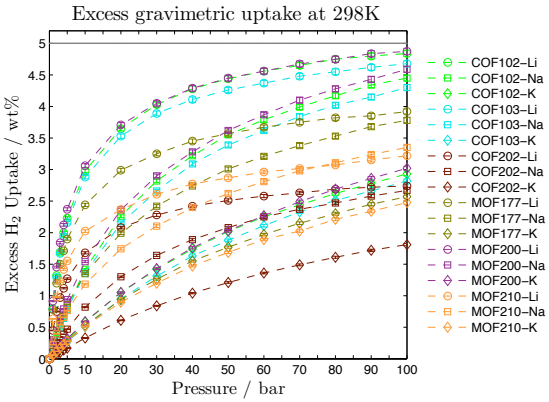
Figure S 12: wt% excess of unmetalated and Li-metalated frameworks (note the changes in the y-axis scale)



13.1: All metalated COFs

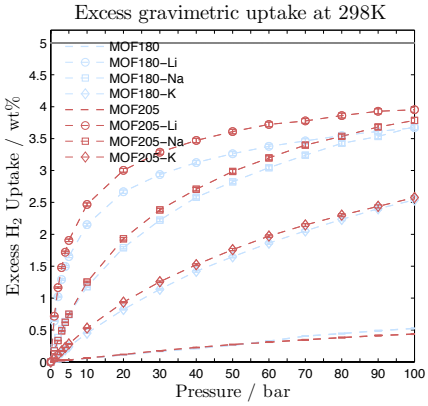


13.2: All metalated MOFs



13.3: All metalated wt% exc.

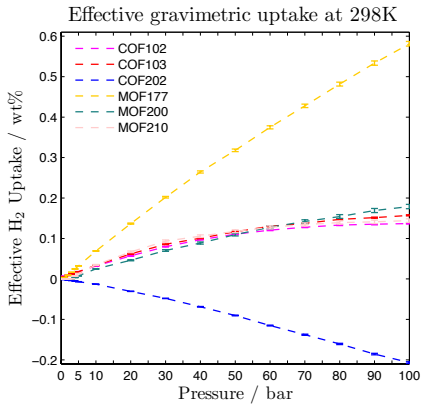
Figure S13: wt% excess of Li-,Na-,K-metalated frameworks



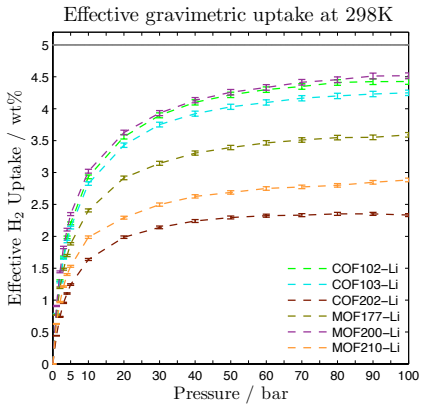
14.1: MOF180 and MOF205

Figure S 14: Wt% excess of Li-,Na-,K-metalated and unmetalated MOF180 and MOF205

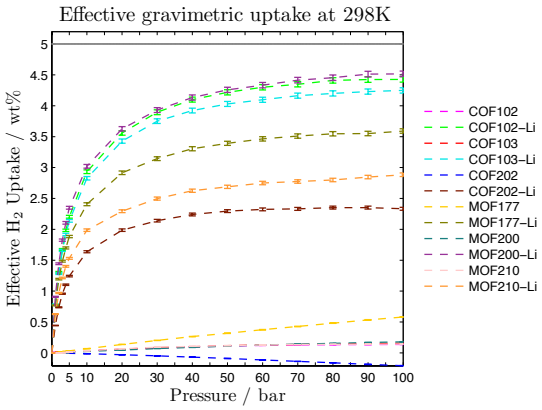
3.4 Effective gravimetric uptake (wt% excess)



15.1: Unmetalated wt% effective

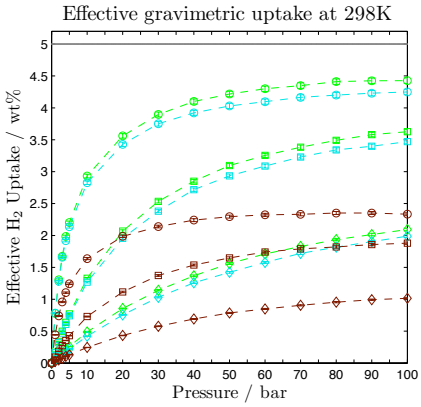


15.2: Li-metalated wt% effective

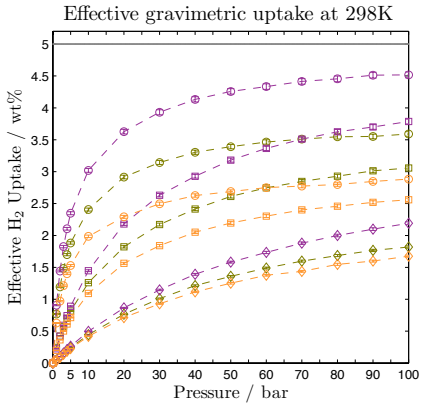


15.3: All wt% effective

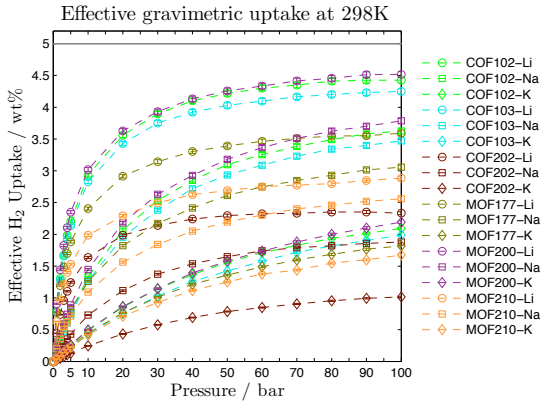
Figure S15: wt% effective of unmetalated and Li-metalated frameworks (note the changes in the y-axis scale)



16.1: All metalated COFs

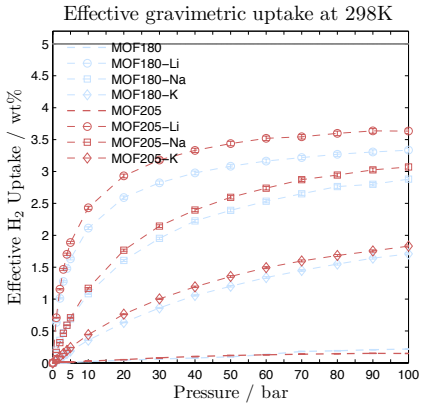


16.2: All metalated MOFs



16.3: All metalated wt% effective

Figure S16: Wt% effective of Li-,Na-,K-metalated frameworks

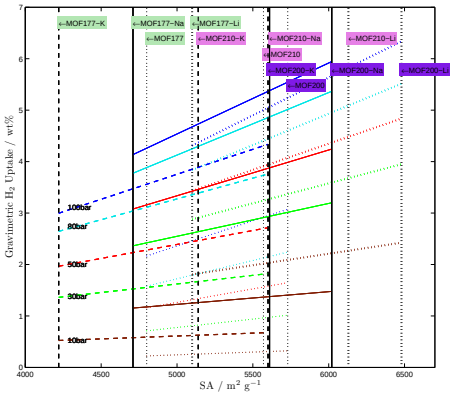


17.1: MOF180 and MOF205

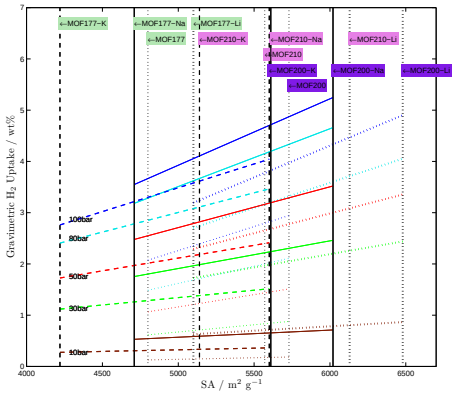
Figure S17: Wt% effective of Li-,Na-,K-metalated and unmetalated MOF180 and MOF205

4 SA vs Grav. Delivery & Vp vs Grav. Delivery

4.1 SA vs Grav. Delivery for MOFs



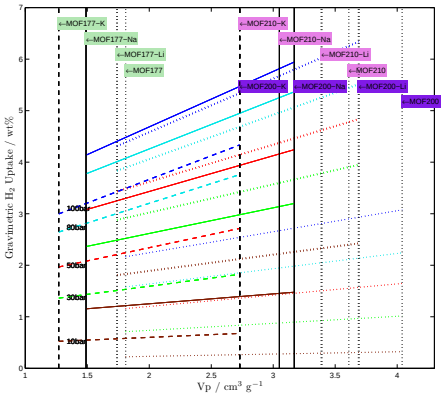
18.1: Basis = 1 bar



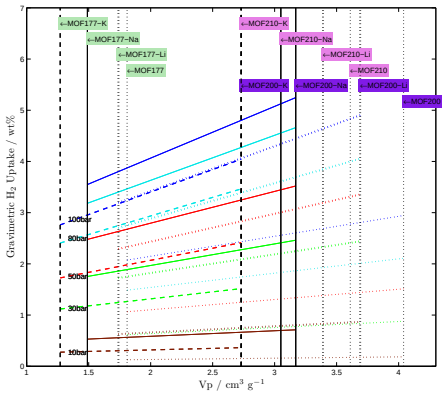
18.2: Basis = 5 bar

Figure S18: SA vs wt% delivery with basis 1 bar and 5 bar

4.2 Vp vs Grav. Delivery for MOFs



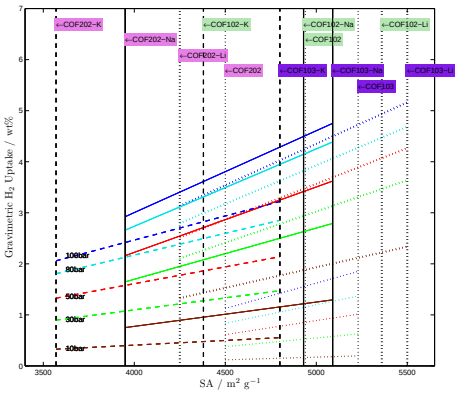
19.1: Basis = 1 bar



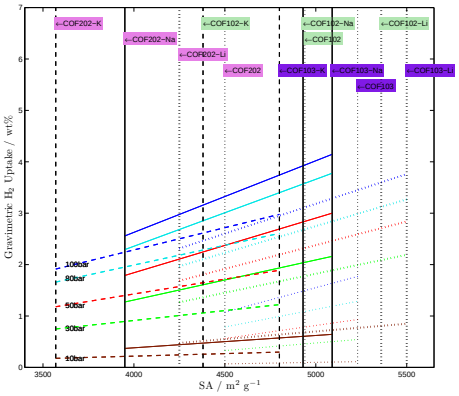
19.2: Basis = 5 bar

Figure S19: Vp vs wt% delivery with basis 1 bar and 5 bar

4.3 SA vs Grav. Delivery for COFs



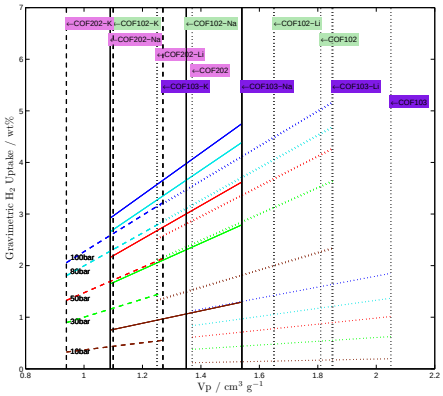
20.1: Basis = 1 bar



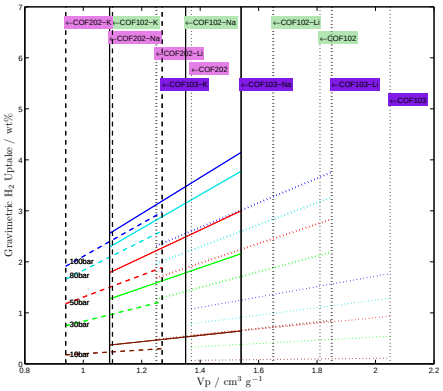
20.2: Basis = 5 bar

Figure S20: SA vs wt% delivery with basis 1 bar and 5 bar

4.4 Vp vs Grav. Delivery for COFs



21.1: Basis = 1 bar

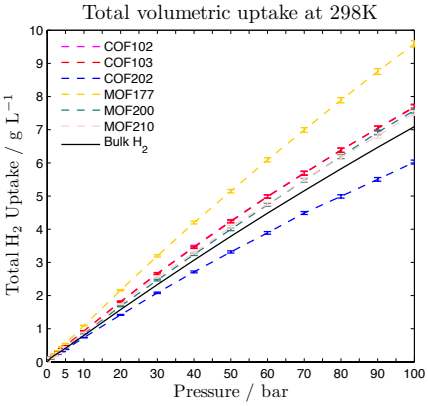


21.2: Basis = 5 bar

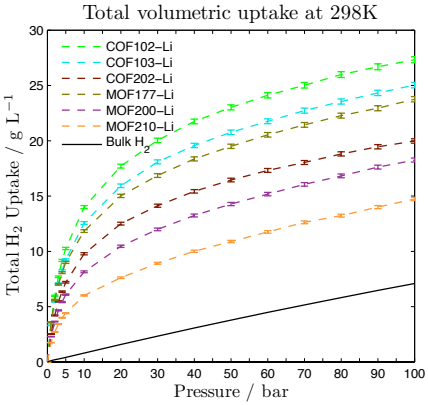
Figure S21: Vp vs wt% delivery with basis 1 bar and 5 bar

5 Volumetric uptake

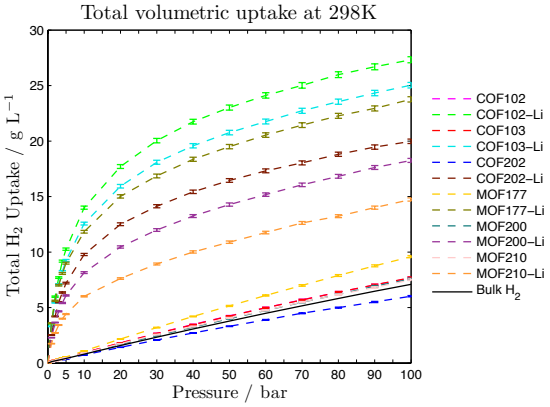
5.1 Total volumetric uptake (g H_2/L)



22.1: Unmetalated total vol.

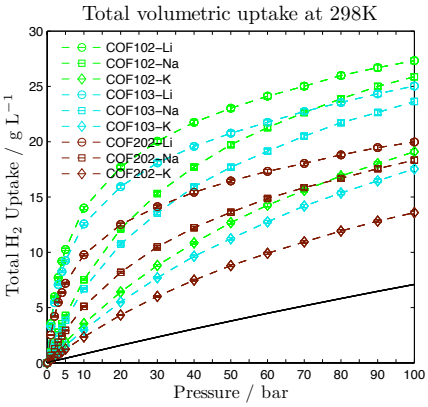


22.2: Metalated total vol.

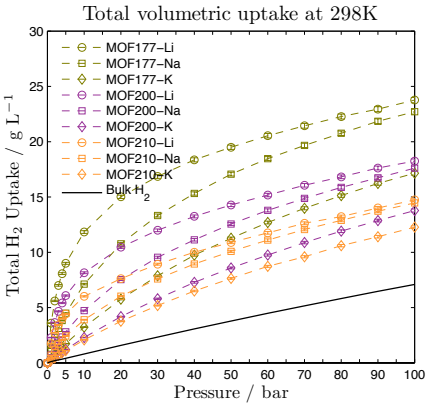


22.3: All total vol.

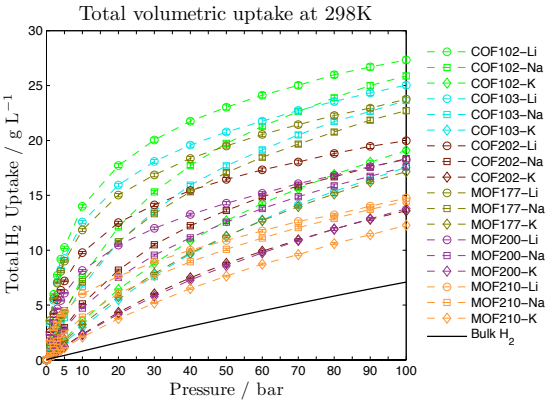
Figure S22: Total vol. of unmetalated and Li-metalated frameworks (note the changes in the y-axis scale). Bulk H_2 is shown for comparison.



23.1: All metalated COFs

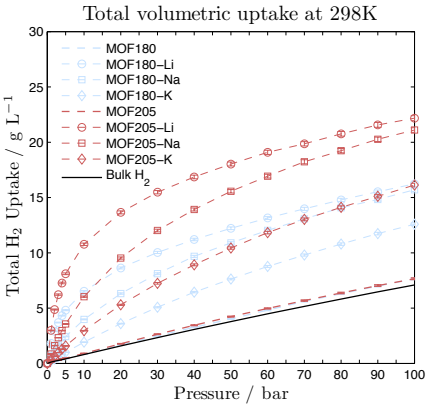


23.2: All metalated MOFs



23.3: All metalated vol. tot.

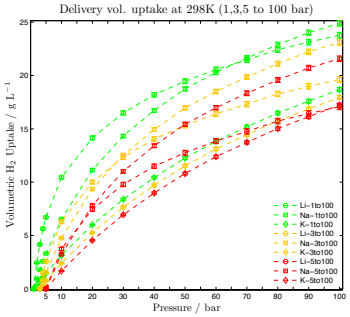
Figure S23: Volumetric total of Li-,Na-,K-metalated frameworks. Bulk H_2 is shown for comparison.



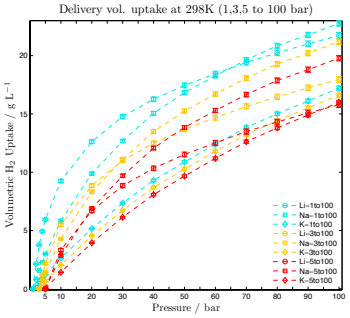
24.1: MOF180 and MOF205

Figure S 24: Vol. total of Li-,Na-,K-metalated and unmetalated MOF180 and MOF205. Bulk H_2 is shown for comparison.

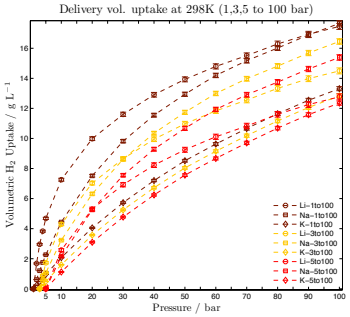
5.2 Delivery volumetric uptake (g H_2/L)



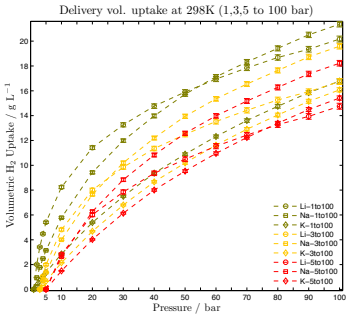
25.1: COF102 delivery vol.



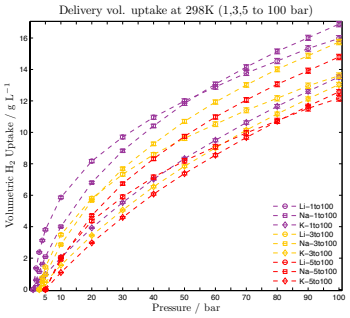
25.2: COF103 delivery vol.



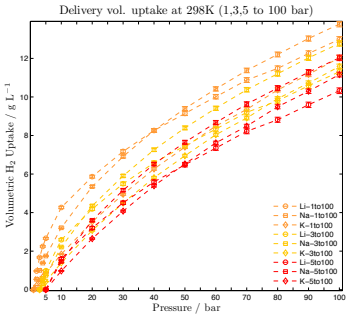
25.3: COF202 delivery vol.



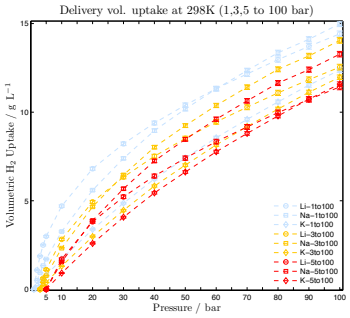
25.4: MOF177 delivery vol.



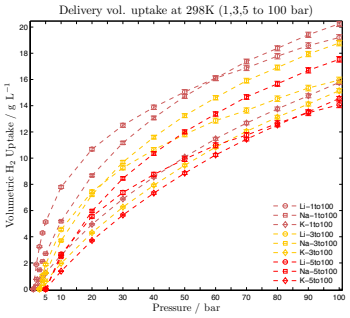
25.5: MOF200 delivery vol.



25.6: MOF210 delivery vol.

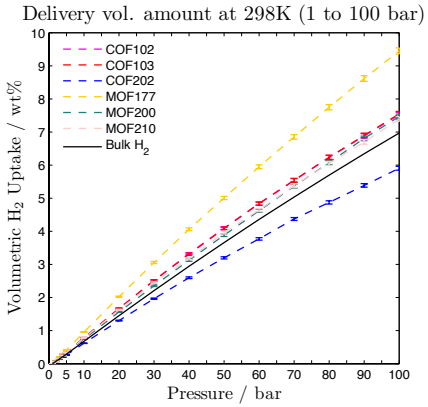


25.7: MOF180 delivery vol.

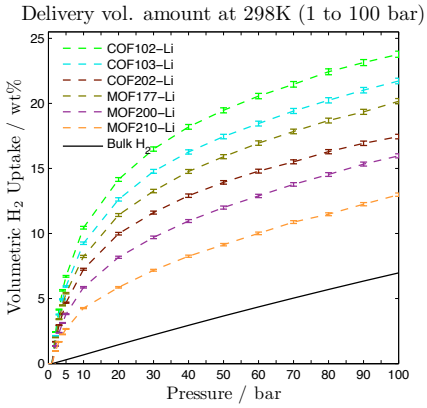


25.8: MOF205 delivery vol.

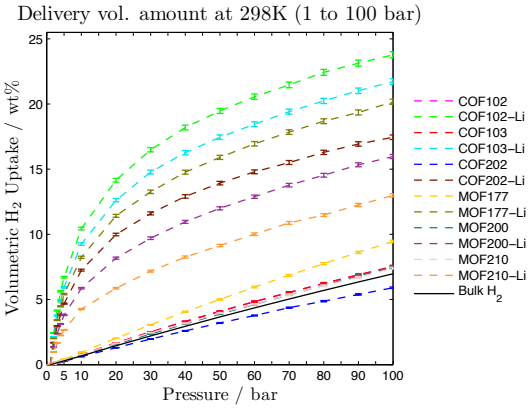
Figure S25: Delivery vol. of unmetalated and Li-,Na-,K-metalated frameworks at different references (1 to 100 bar, 3 to 100 bar & 5 to 100 bar) (note the changes in the y-axis scale)



26.1: Unmetalated delivery vol. (1 to 100 bar)

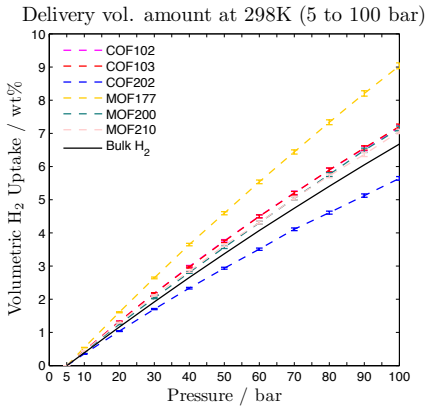


26.2: Metalated delivery vol. (1 to 100 bar)

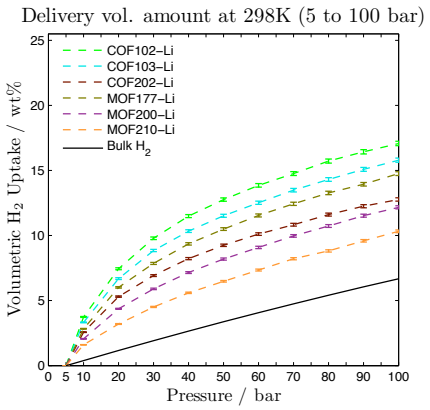


26.3: All delivery vol. (1 to 100 bar)

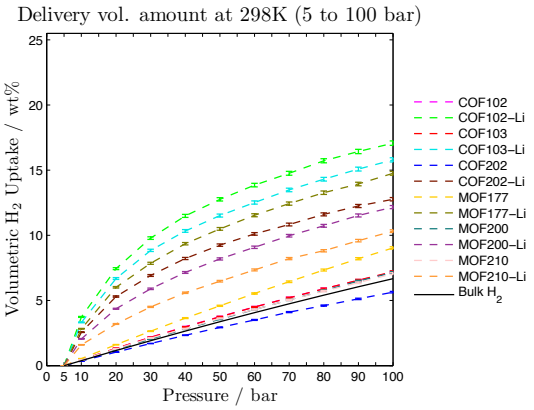
Figure S26: Delivery vol. of unmetalated and Li-metalated frameworks (note the changes in the y-axis scale). Bulk H_2 is shown for comparison. The reference is 1 bar.



27.1: Unmetalated delivery vol. (5 to 100 bar)

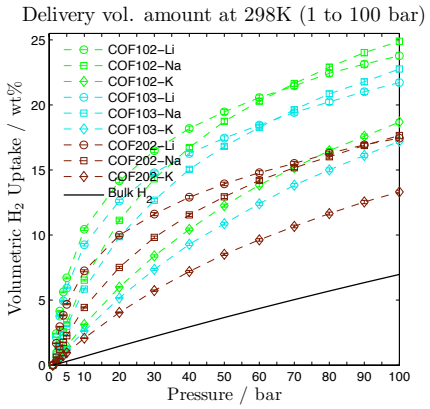


27.2: Metalated delivery vol. (5 to 100 bar)

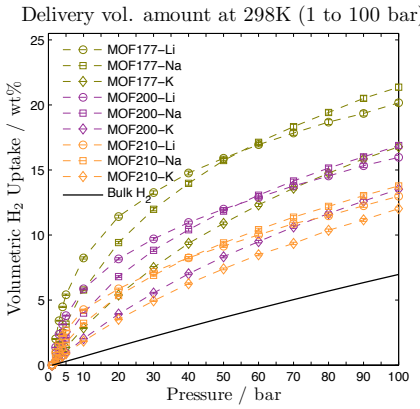


27.3: All delivery vol. (5 to 100 bar)

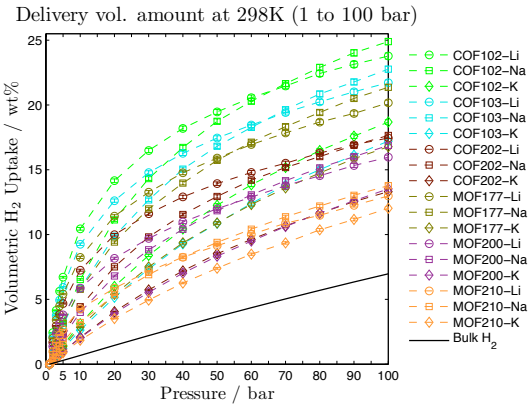
Figure S27: Delivery vol. of unmetalated and Li-metalated frameworks (note the changes in the y-axis scale). Bulk H_2 is shown for comparison. The reference is 5 bar.



28.1: All metalated COFs (1 to 100 bar)

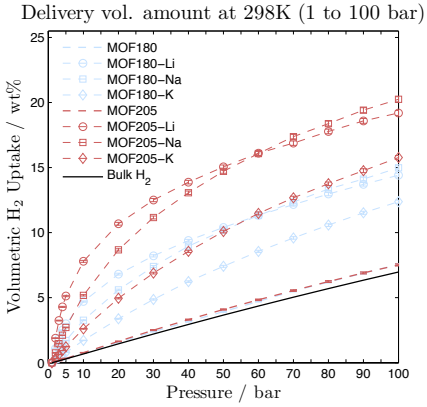


28.2: All metalated MOFs (1 to 100 bar)



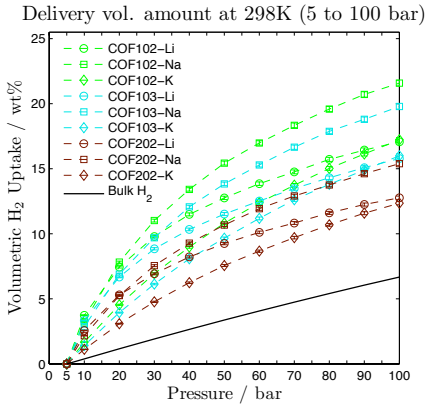
28.3: All metalated vol. delivery (1 to 100 bar)

Figure S28: Volumetric delivery of Li-,Na-,K-metalated frameworks. Bulk H_2 is shown for comparison. The reference is 1 bar.

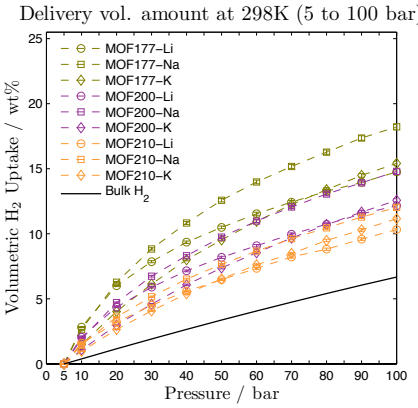


29.1: MOF180 and MOF205 (1 to 100 bar)

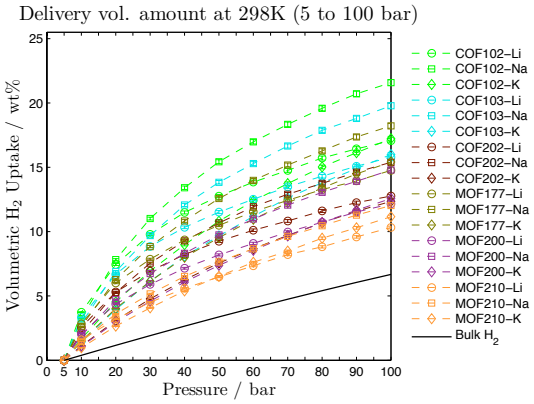
Figure S29: Vol. delivery of Li-,Na-,K-metalated and unmetalated MOF180 and MOF205. Bulk H_2 is shown for comparison. The reference is 1 bar.



30.1: All metalated COFs (5 to 100 bar)

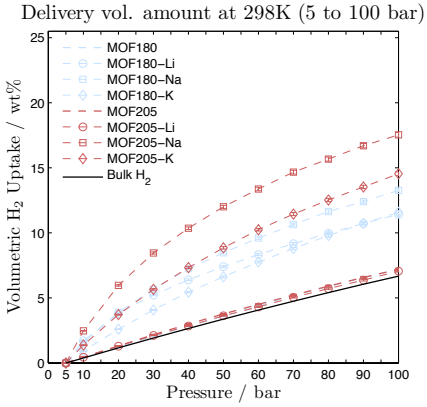


30.2: All metalated MOFs (5 to 100 bar)



30.3: All metalated vol. delivery (5 to 100 bar)

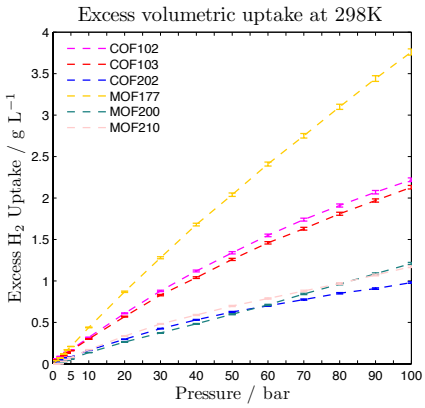
Figure S30: Volumetric delivery of Li-,Na-,K-metalated frameworks. Bulk H_2 is shown for comparison. The reference is 5 bar.



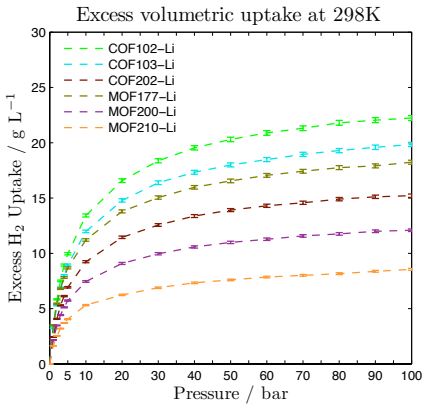
31.1: MOF180 and MOF205 (5 to 100 bar)

Figure S31: Vol. delivery of Li-,Na-,K-metalated and unmetalated MOF180 and MOF205. Bulk H_2 is shown for comparison. The reference is 5 bar.

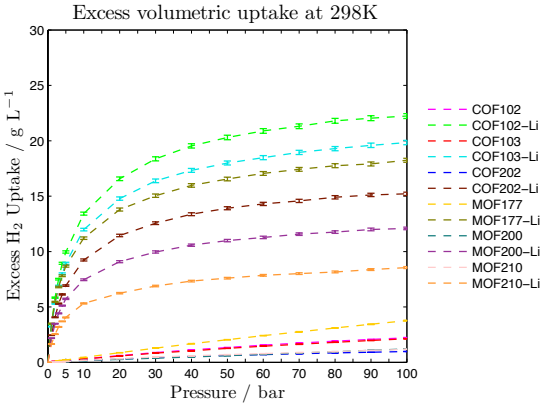
5.3 Excess volumetric uptake (g H_2/L)



32.1: Unmetalated excess vol.

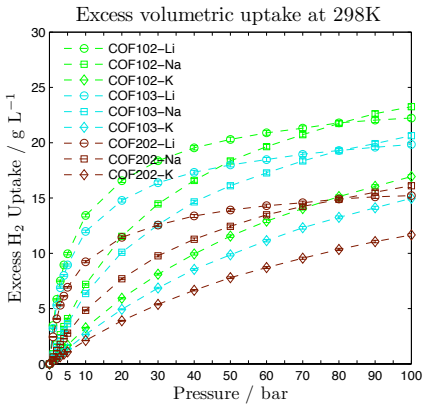


32.2: Metalated excess vol.

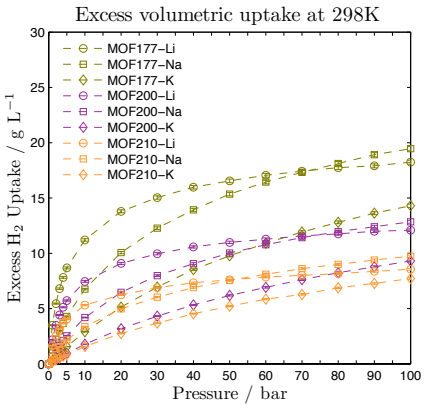


32.3: All excess vol.

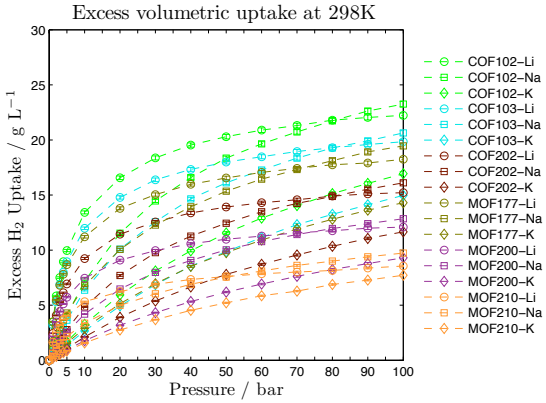
Figure S 32: Excess vol. of unmetalated and Li-metalated frameworks (note the changes in the y-axis scale). Bulk H_2 is not shown for comparison because we are cosidering excess volumetric units, as it is shown in eqn.1, so putting the vol. H_2 here would be meaningless.



33.1: All metalated COFs

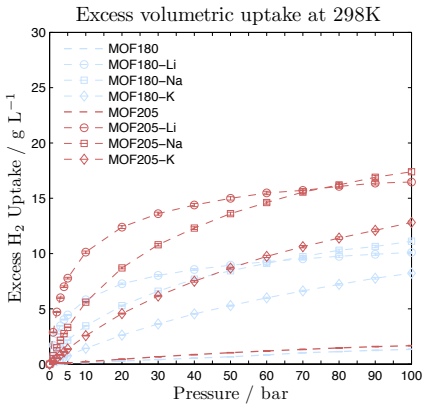


33.2: All metalated MOFs



33.3: All metalated vol. exc.

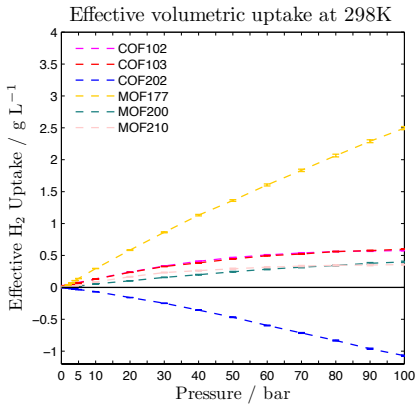
Figure S33: Volumetric excess of Li-,Na-,K-metalated frameworks. Bulk H_2 is not shown for comparison because we are cosidering excess volumetric units, as it is shown in eqn.1.



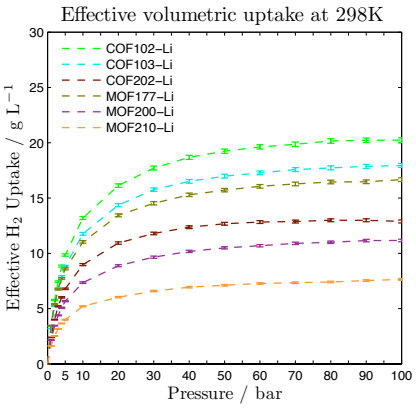
34.1: MOF180 and MOF205

Figure S 34: Vol. excess of Li-,Na-,K-metalated and unmetalated MOF180 and MOF205. Bulk H_2 is not shown for comparison because we are cosidering excess volumetric units, as it is shown in eqn.1.

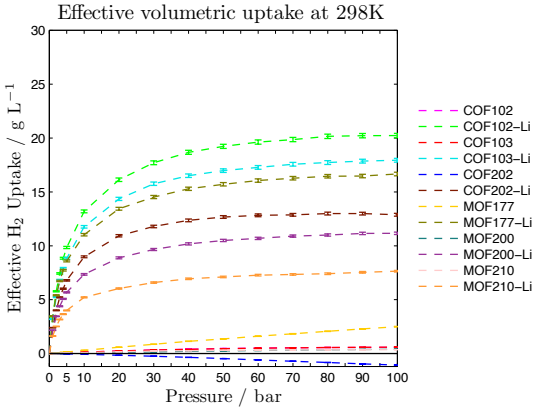
5.4 Effective volumetric uptake (g H_2/L)



35.1: Unmetalated effective vol.

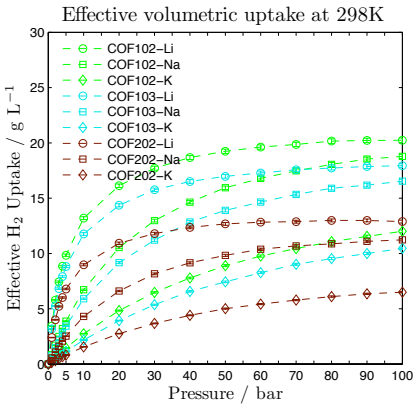


35.2: Metalated effective vol.

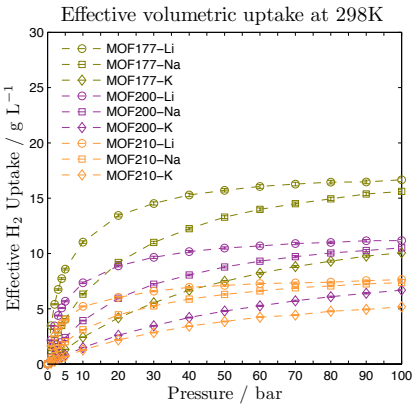


35.3: All effective vol.

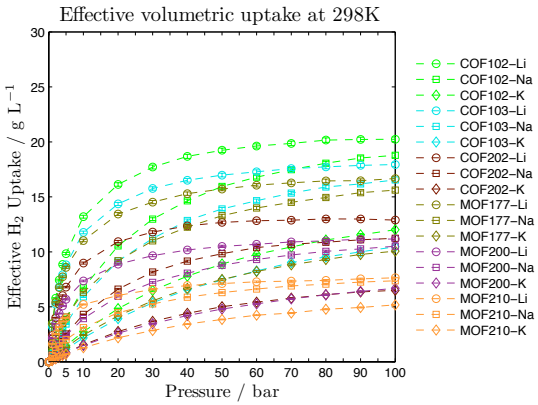
Figure S35: Effective vol. of unmetalated and Li-metalated frameworks (note the changes in the y-axis scale). Bulk H_2 is not shown for comparison because we are cosidering effective volumetric units, as it is shown in eqn.2, so putting the vol. H_2 herre would be meaningless.



36.1: All metalated COFs

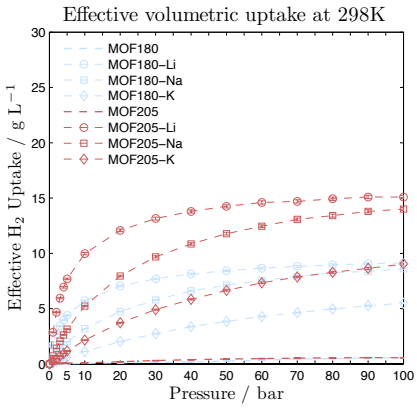


36.2: All metalated MOFs



36.3: All metalated vol. effective

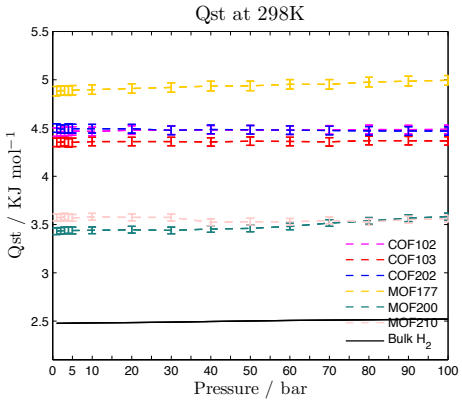
Figure S36: Volumetric effective of Li-,Na-,K-metalated frameworks. Bulk H_2 is not shown for comparison because we are cosidering effective volumetric units, as it is shown in eqn.2.



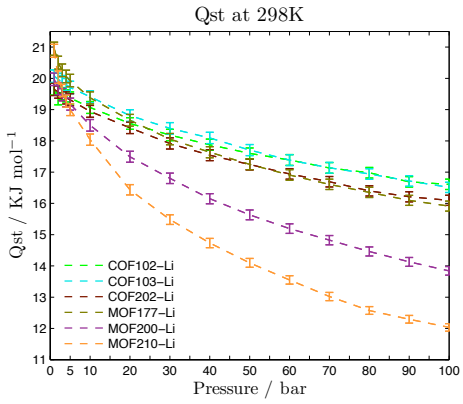
37.1: MOF180 and MOF205

Figure S37: Vol. effective of Li-,Na-,K-metalated and unmetalated MOF180 and MOF205. Bulk H_2 is not shown for comparison because we are cosidering effective volumetric units, as it is shown in eqn.2.

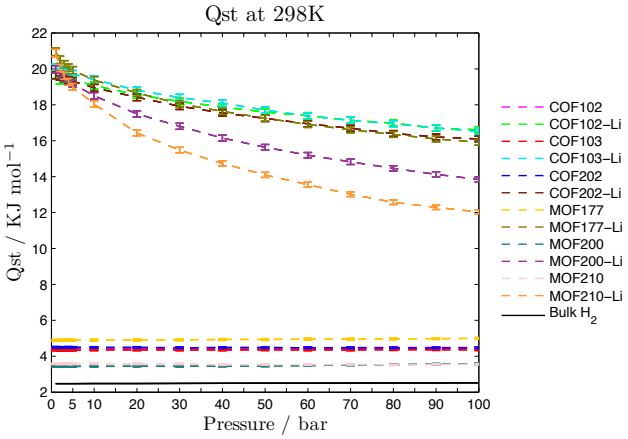
6 Heat of adsorption (Qst)



38.1: Unmetalated Qst

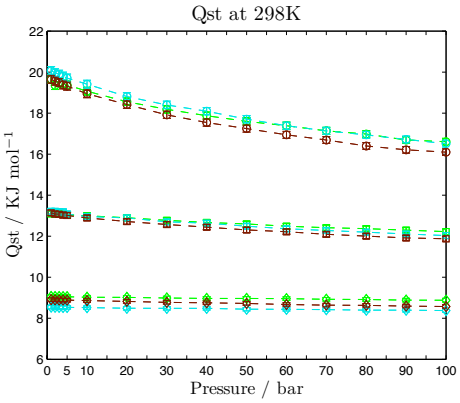


38.2: Metalated Qst

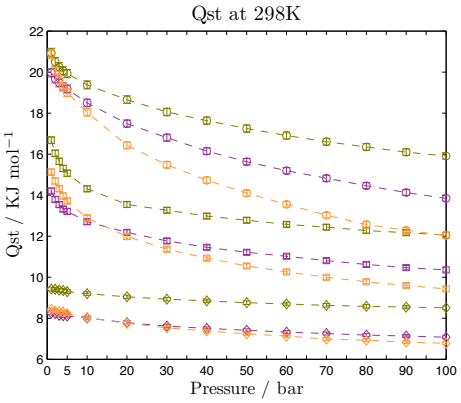


38.3: All frameworks' Qst

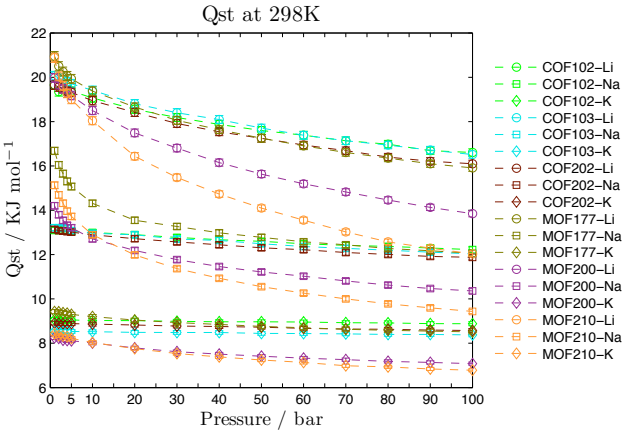
Figure S38: Qst of unmetalated and Li-metalated frameworks (note the changes in the y-axis scale)



39.1: All metalated COFs

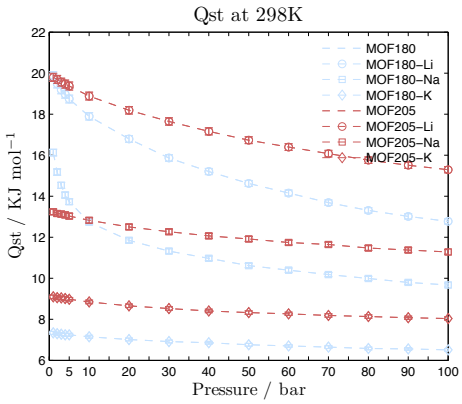


39.2: All metalated MOFs



39.3: All metalated frameworks

Figure S39: Qst of Li-,Na-,K-metalated frameworks

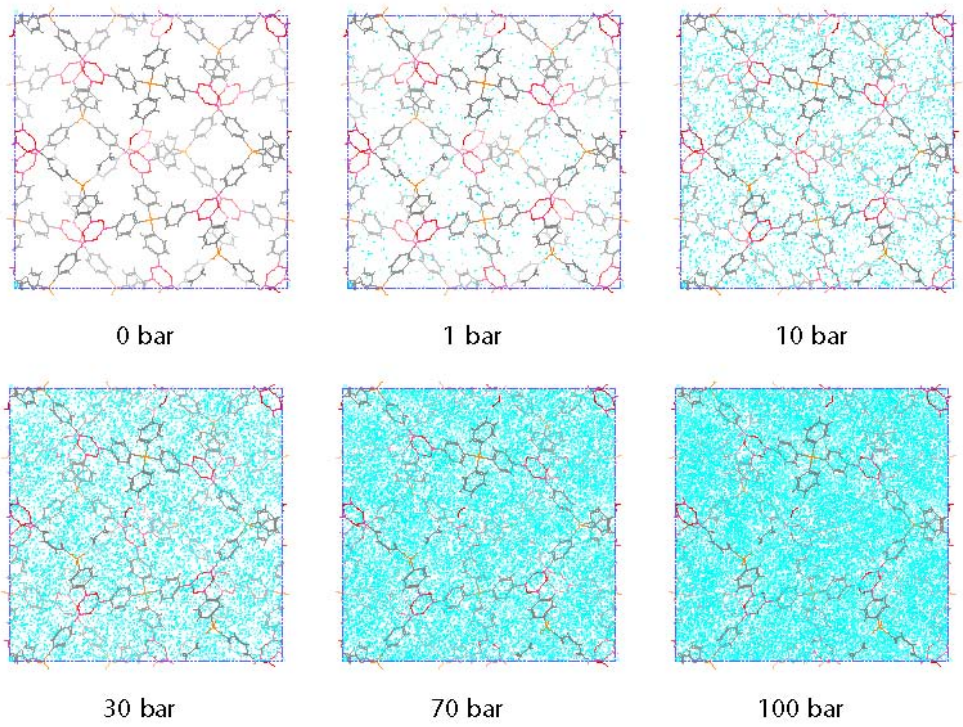


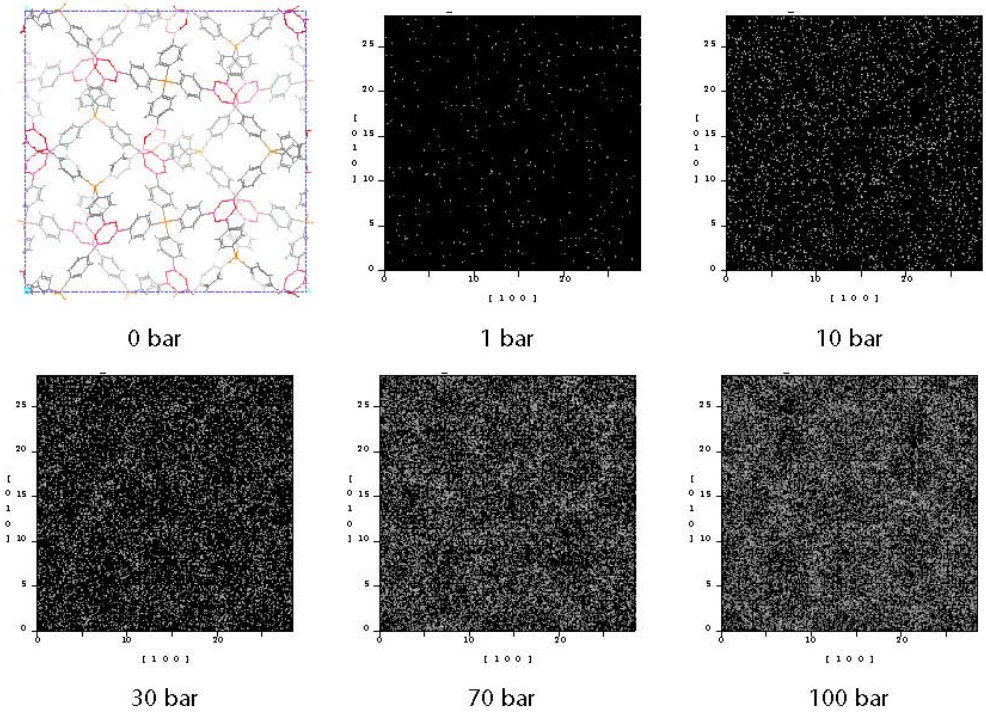
40.1: MOF180 and MOF205

Figure S40: Qst. of Li-,Na-,K-metalated and unmetalated MOF180 and MOF205.

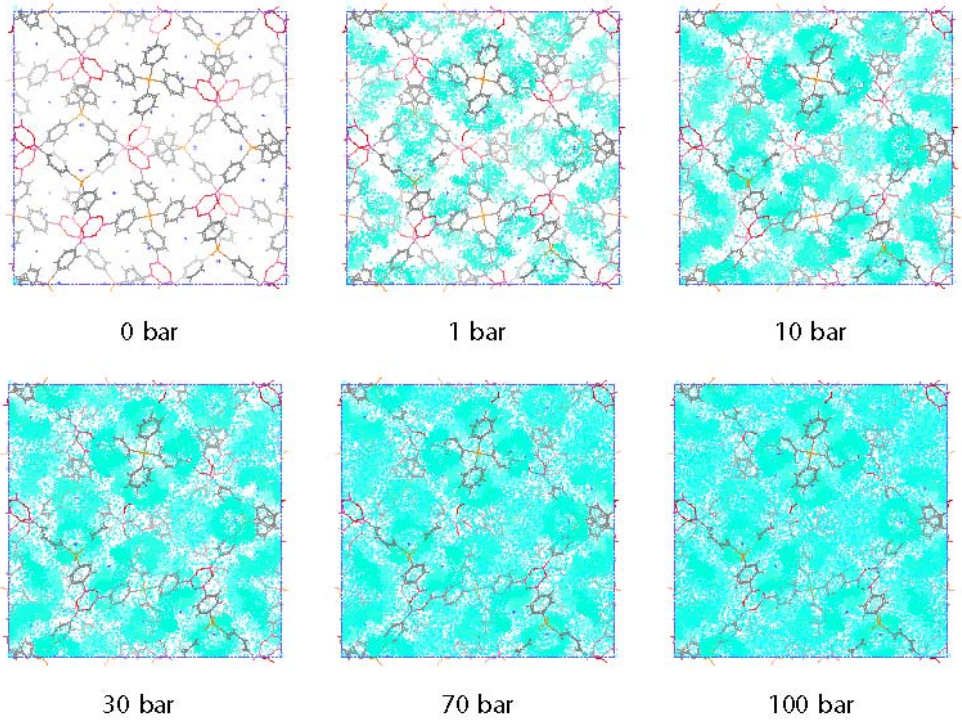
7 Mechanism

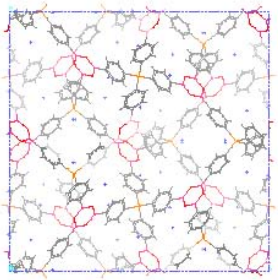
7.1 COF103 at 298K



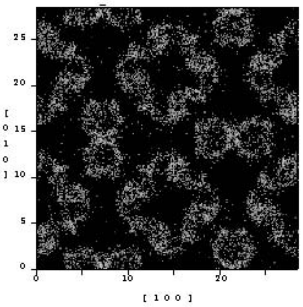

0 bar
1 bar
10 bar
30 bar
70 bar
100 bar

7.2 COF103-Li at 298K

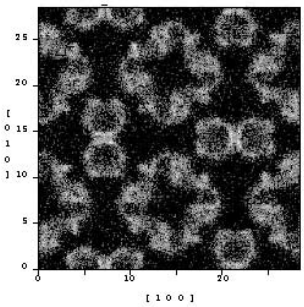




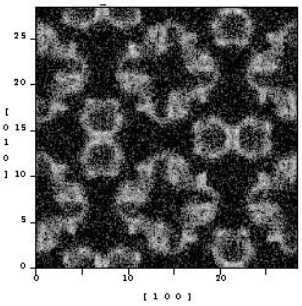
0 bar



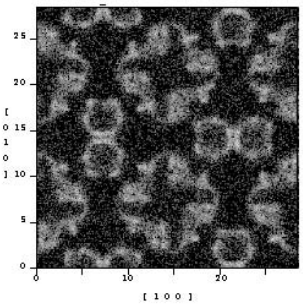
1 bar



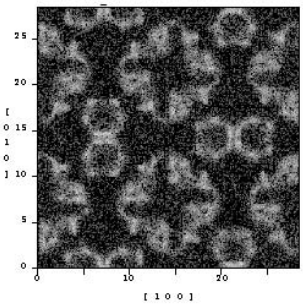
10 bar



30 bar

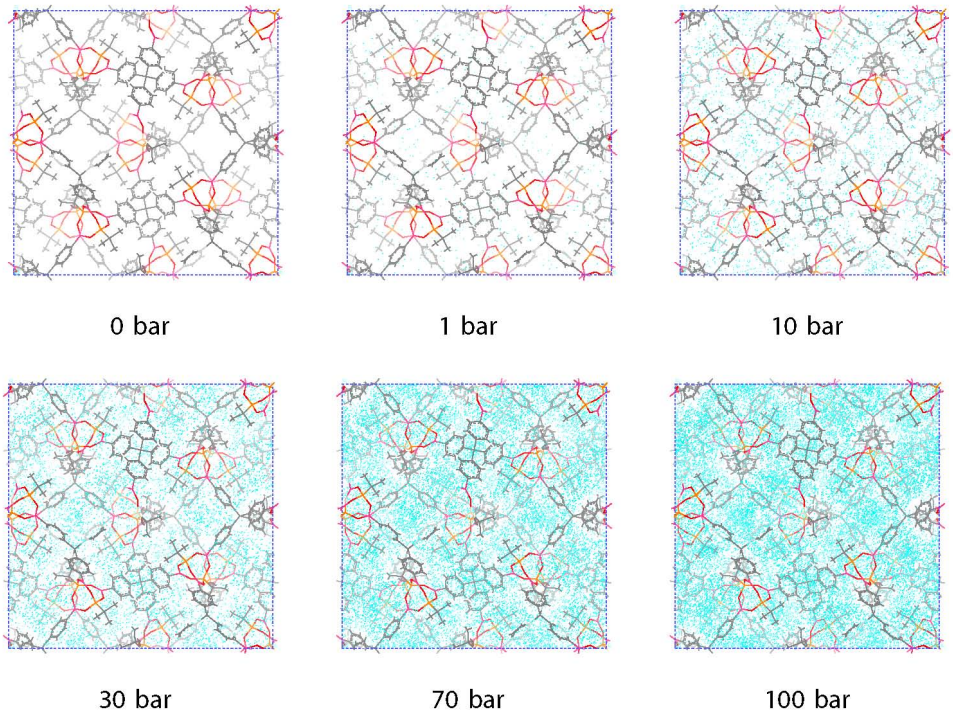


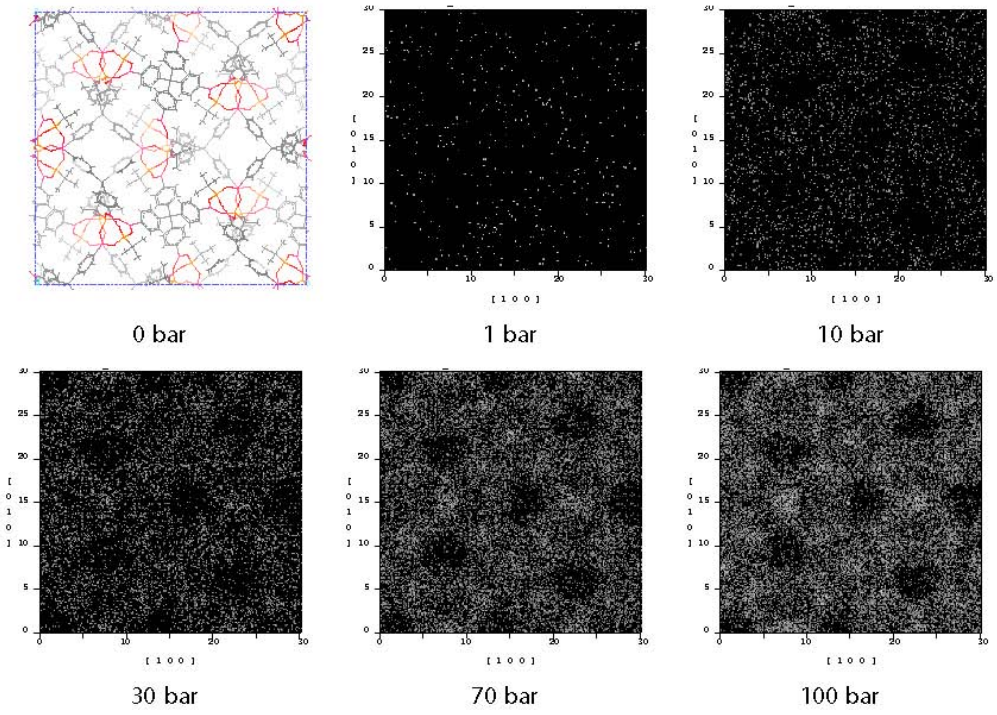
70 bar



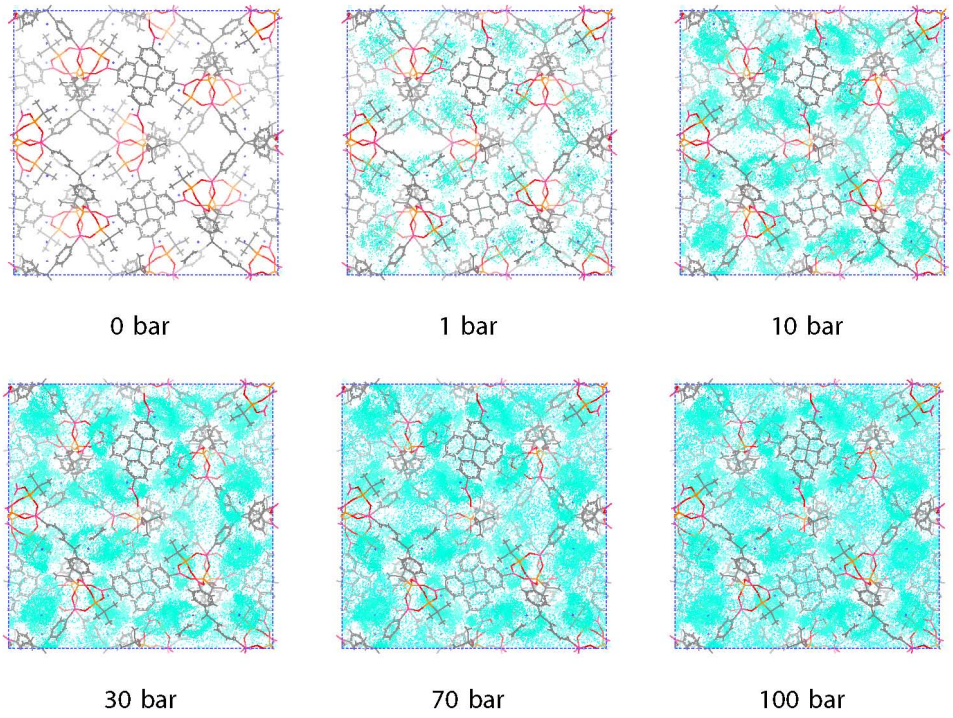
100 bar

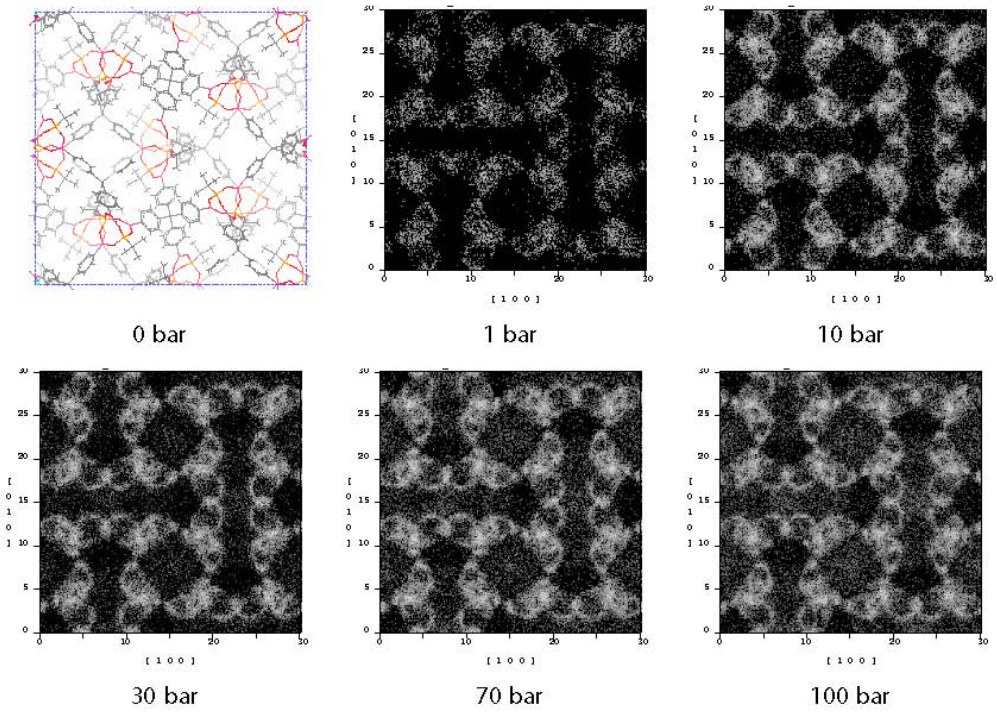
7.3 COF202 at 298K



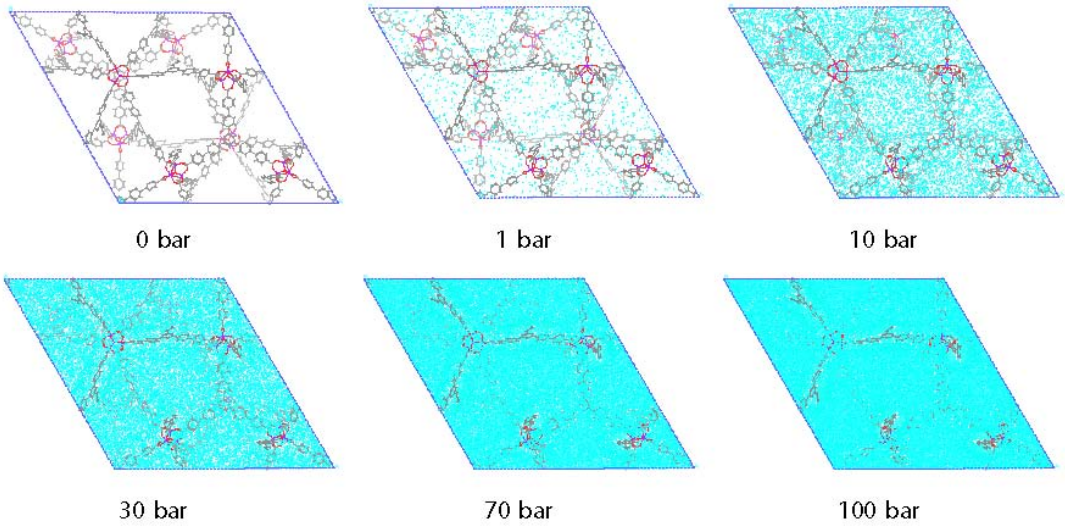

0 bar
1 bar
10 bar
30 bar
70 bar
100 bar

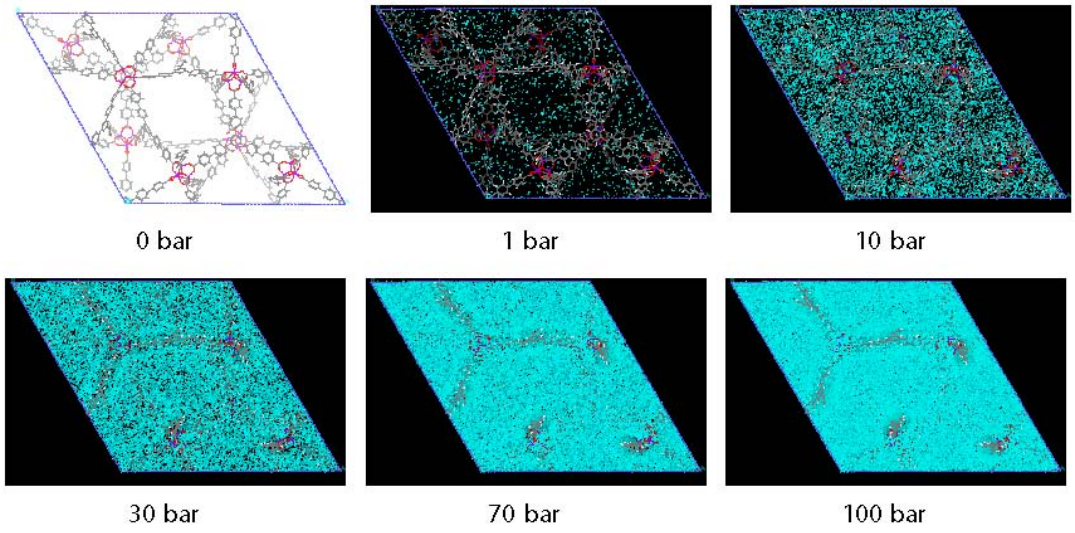
7.4 COF202-Li at 298K



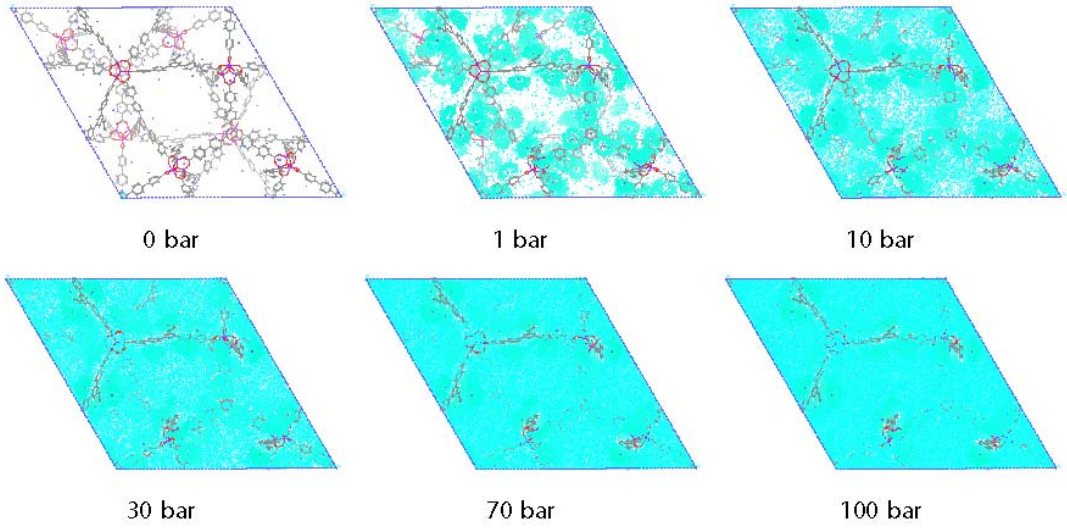

0 bar
1 bar
10 bar
30 bar
70 bar
100 bar

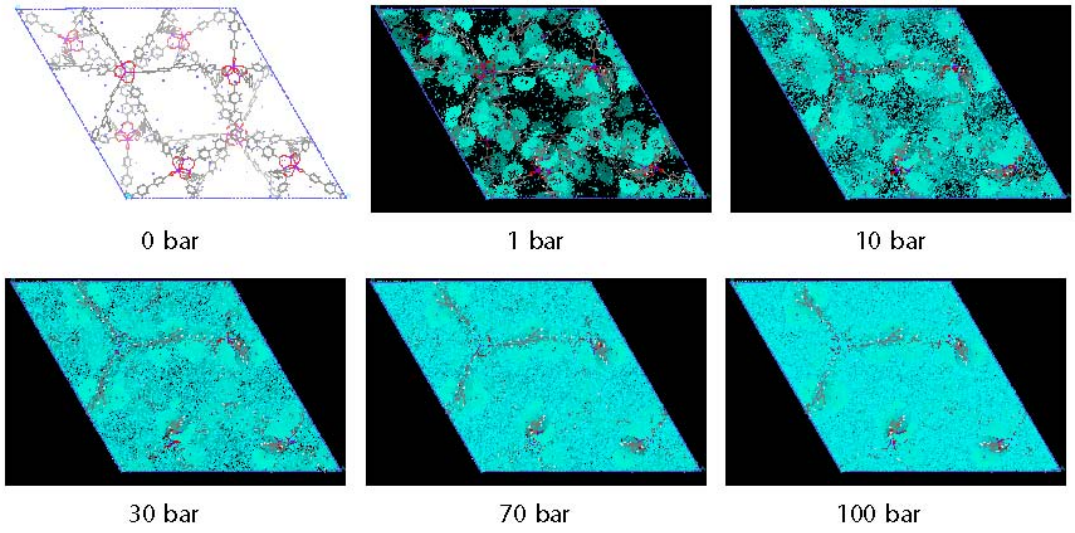
7.5 MOF200 at 298K



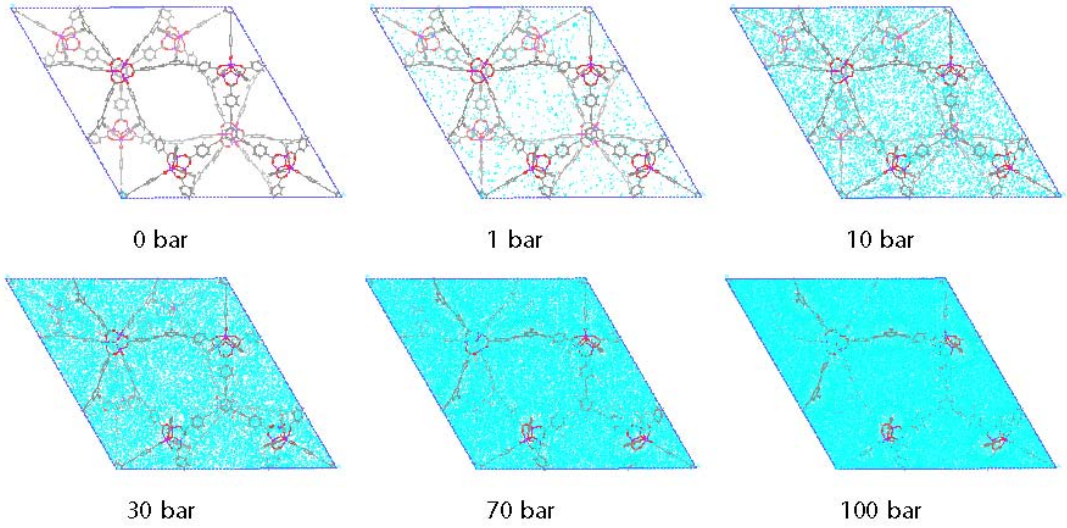

0 bar
1 bar
10 bar
30 bar
70 bar
100 bar

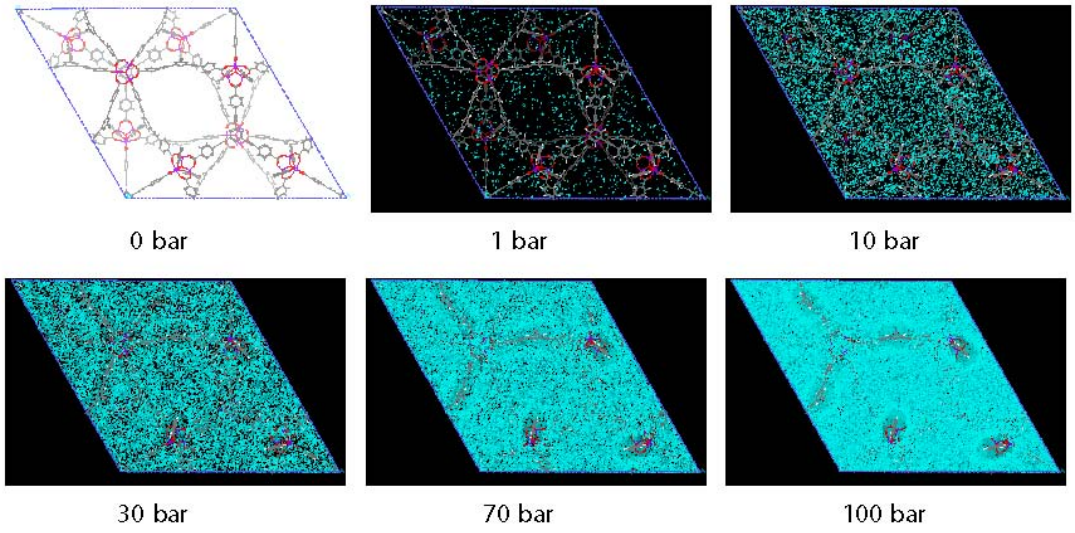
7.6 MOF200-Li at 298K



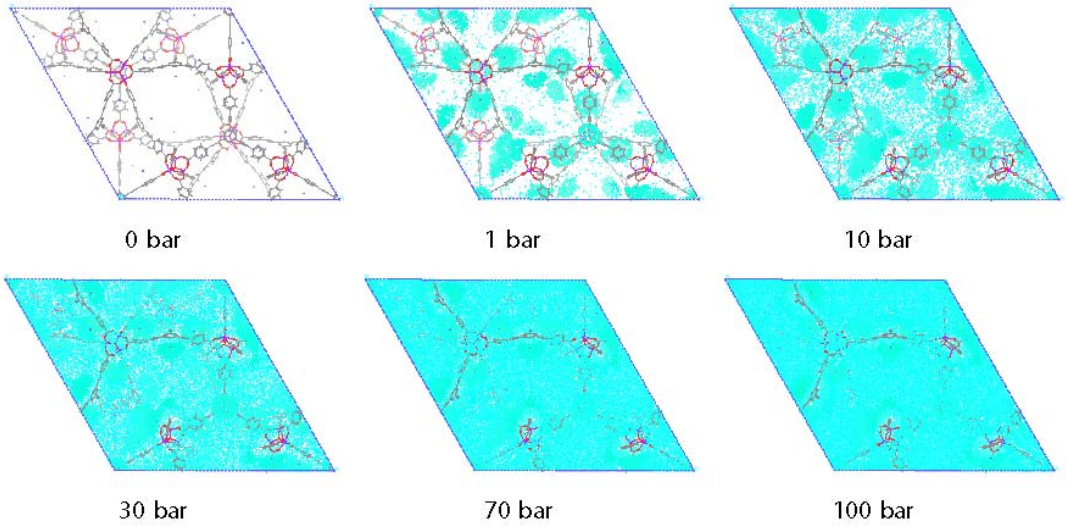

0 bar
1 bar
10 bar
30 bar
70 bar
100 bar

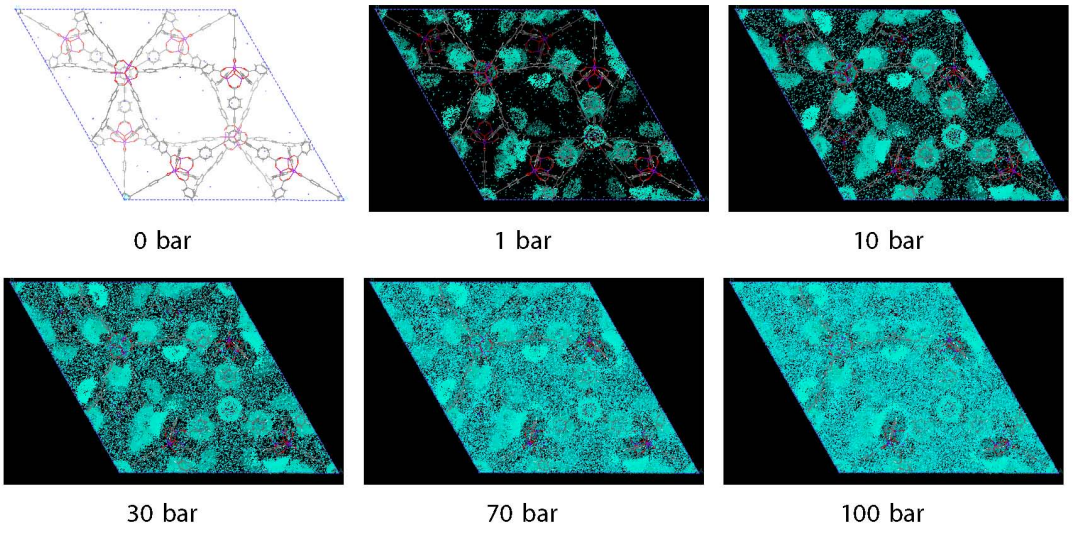
7.7 MOF180 at 298K




0 bar
1 bar
10 bar
30 bar
70 bar
100 bar

7.8 MOF180-Li at 298K




0 bar
1 bar
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30 bar
70 bar
100 bar

8 Coordinates for metalated MOFs and COFs

We present only the coordinates of the Li-metalated frameworks in this supplementary material. The Na and K analogs can be easily derived from these coordinates coordinates with the minimization procedure described in the main text.

For COFs, the Li-metalated structures are reported with their highest symmetrical space group as reported on the literature since we were able to optimize them with these constrains.

For MOF177,MOF200,MOF180, MOF205, we report the coordinates with the P1 space group because when using the X-ray experimental coordinates there is some termal disorder that we removed. Thus we have reduced the symmetry to obtain a single position for the ligands. For MOF210, we were able to keep the highest symmetrical group and this simplified greatly our calculations.

8.1 COF102-Li

```
Name
COF102-Li

Space group symmetry
I -4 3 d
a = b = c = 27.408 A
 alpha = betha = gamma = 90.000
```

Atom	x	y	z
C1	0.37500	0.00000	0.25000
C2	0.33956	0.06887	0.19425
H3	0.36296	0.05892	0.16423
C4	0.34041	0.04366	0.23931
C5	0.30513	0.05691	0.27459
H6	0.30333	0.03769	0.30908
C7	0.27244	0.09511	0.26632
H8	0.24648	0.10447	0.29462
C9	0.27378	0.12114	0.22238
B10	0.23795	0.16478	0.21336
C11	0.30737	0.10758	0.18638
H12	0.30839	0.12639	0.15162
O13	0.24705	0.19714	0.17186
Li14	0.36172	0.23764	0.59667

8.2 COF103-Li

```
Name
COF103-Li

Space group symmetry
I -4 3 d
a = b = c = 28.455 A
 alpha = betha = gamma = 90.000
```

Atom	x	y	z
Si1	0.37500	0.00000	0.25000
C2	0.34090	0.07986	0.20018
H3	0.36784	0.07277	0.17437
C4	0.33593	0.05142	0.24010
C5	0.30010	0.06115	0.27245
H6	0.29550	0.03927	0.30325
C7	0.26983	0.09915	0.26528
H8	0.24245	0.10590	0.29087
C9	0.27505	0.12797	0.22557
B10	0.24113	0.17063	0.21742
C11	0.31085	0.11805	0.19309
H12	0.31554	0.13955	0.16202
O13	0.20185	0.17749	0.24990
Li14	0.38087	0.25366	0.58365

8.3 COF202-Li

```
Name
COF202-Li

Space group symmetry
I -4 3 d
a = b = c = 29.927 A
 alpha = betha = gamma = 90.000
```

Atom	x	y	z
Si1	0.37500	0.00000	0.25000
Si2	0.73963	0.73963	0.73963
C3	0.82204	0.77389	0.75460
O4	0.74018	0.76138	0.69121
B5	0.71850	0.74996	0.64963
O6	0.68931	0.71236	0.64158
C7	0.66633	0.62128	0.59801
H8	0.83675	0.74046	0.75431
H9	0.84328	0.79506	0.77542
H10	0.67869	0.64874	0.57735
H11	0.69495	0.60127	0.60871
H12	0.64546	0.60013	0.57680
Si13	0.67242	0.67242	0.67242
C14	0.63894	0.63894	0.63894
C15	0.77312	0.77312	0.77312
H16	0.82324	0.78719	0.72061
C17	0.65810	0.54060	0.25769
C18	0.68608	0.53981	0.29551
C19	0.71723	0.57438	0.30245
C20	0.72040	0.60974	0.27158
C21	0.69242	0.61053	0.23376
C22	0.66127	0.57596	0.22682
H23	0.73754	0.57381	0.32992
H24	0.69472	0.63620	0.21134
H25	0.68378	0.51413	0.31793
H26	0.64095	0.57653	0.19936
Li27	0.70133	0.63062	0.38085

8.4 MOF177-Li

```
Name
MOF177-Li

Space group symmetry
P 1

 a      b      c
 37.072 37.072 30.033  A

 alpha   betha   gamma
 90.000  90.000  120.000
```

Atom	x	y	z
C1	0.71580	0.10510	0.03099
C2	0.70509	0.13323	0.05008
C3	0.69254	0.12964	0.09511
C4	0.68984	0.09611	0.12043
C5	0.69901	0.06668	0.10167
C6	0.71224	0.07188	0.05696
C7	0.68330	0.16124	0.11605
C8	0.70326	0.20308	0.10138
C9	0.69586	0.23274	0.12229
C10	0.66907	0.22176	0.15915
C11	0.64859	0.18006	0.17342
C12	0.65509	0.15020	0.15187
C13	0.69478	0.03044	0.12847
C14	0.66207	0.00954	0.15929
C15	0.65694	0.97430	0.18247
C16	0.68428	0.95880	0.17545
C17	0.71751	0.98027	0.14544
C18	0.72274	0.01553	0.12246
C19	0.73201	0.11097	0.98432
C20	0.76757	0.10798	0.97474
C21	0.78380	0.11452	0.93144
C22	0.76459	0.12362	0.89622
C23	0.72857	0.12594	0.90559
C24	0.71269	0.12004	0.94916
C25	0.78318	0.13236	0.85059
C26	0.66505	0.25388	0.18518
C27	0.67735	0.91960	0.19752
C28	0.88635	0.11634	0.75012
C29	0.70794	0.35029	0.74863

C30	0.68626	0.30650	0.74883
C31	0.70940	0.28323	0.74927
C32	0.69429	0.24555	0.72576
C33	0.71611	0.22383	0.72614
C34	0.75392	0.23970	0.74930
C35	0.77732	0.21711	0.74913
H36	0.70714	0.15824	0.02970
H37	0.68182	0.09342	0.15536
H38	0.71903	0.04944	0.04176
H39	0.72577	0.21353	0.07462
H40	0.71254	0.26472	0.11083
H41	0.62751	0.17048	0.20155
H42	0.63793	0.11840	0.16365
H43	0.63962	0.01967	0.16461
H44	0.63092	0.95861	0.20517
H45	0.73944	0.96960	0.13933
H46	0.74884	0.03113	0.09986
H47	0.78343	0.10142	1.00107
H48	0.81159	0.11255	0.92559
H49	0.71309	0.13311	0.87937
H50	0.68511	0.12229	0.95534
H51	0.74164	0.36706	0.74876
H52	0.66592	0.23307	0.70642
H53	0.70377	0.19499	0.70761
C54	0.23031	0.11894	0.74820
C55	0.68658	0.37267	0.74829
C56	0.64282	0.35059	0.74802
C57	0.62040	0.30683	0.74810
C58	0.64247	0.28510	0.74855
H59	0.62548	0.25141	0.74869
C60	0.57400	0.28397	0.74791
C61	0.55202	0.29957	0.72406
C62	0.50854	0.27874	0.72477
C63	0.48598	0.24138	0.74852
C64	0.50771	0.22533	0.77180
C65	0.55123	0.24658	0.77186
H66	0.56698	0.23401	0.79131
H67	0.49104	0.19672	0.79068
C68	0.44002	0.21927	0.74898
H69	0.49254	0.29157	0.70614
H70	0.56836	0.32770	0.70440
H71	0.62612	0.36758	0.74776
C72	0.70986	0.41905	0.74827
C73	0.74752	0.44140	0.72466
C74	0.76938	0.48493	0.72485

C75	0.75368	0.50707	0.74790
C76	0.71600	0.48492	0.77124
C77	0.69456	0.44143	0.77181
H78	0.66622	0.42541	0.79120
H79	0.70343	0.50125	0.78970
C80	0.77643	0.55303	0.74775
H81	0.79823	0.50127	0.70629
H82	0.75987	0.42532	0.70544
C83	0.74701	0.29865	0.77301
C84	0.76922	0.27735	0.77262
H85	0.79809	0.29005	0.79117
H86	0.75917	0.32699	0.79236
C87	0.38596	0.10605	0.46762
C88	0.42366	0.13566	0.44772
C89	0.43309	0.13100	0.40342
C90	0.40426	0.09573	0.37902
C91	0.36598	0.06571	0.39797
C92	0.35738	0.07139	0.44242
C93	0.47247	0.16371	0.38222
C94	0.48433	0.20609	0.38549
C95	0.52049	0.23680	0.36434
C96	0.54624	0.22606	0.34008
C97	0.53485	0.18373	0.33767
C98	0.49822	0.15292	0.35809
C99	0.33479	0.02877	0.37144
C100	0.34755	0.00873	0.34077
C101	0.31614	0.97164	0.31601
C102	0.27349	0.95626	0.32333
C103	0.26192	0.97761	0.35373
C104	0.29170	0.01292	0.37698
C105	0.37601	0.11185	0.51441
C106	0.33705	0.10744	0.52494
C107	0.32814	0.11450	0.56839
C108	0.35764	0.12541	0.60275
C109	0.39629	0.12886	0.59247
C110	0.40550	0.12257	0.54875
C111	0.34863	0.13488	0.64835
C112	0.58334	0.25841	0.31535
C113	0.24108	0.91731	0.30103
H114	0.44559	0.16269	0.46667
H115	0.41107	0.09257	0.34465
H116	0.32868	0.04829	0.45799
H117	0.46502	0.21538	0.40358
H118	0.52820	0.26903	0.36682
H119	0.55375	0.17426	0.31904

H120	0.49005	0.12059	0.35519
H121	0.38024	0.01918	0.33580
H122	0.32661	0.95614	0.29323
H123	0.22930	0.96680	0.35991
H124	0.28065	0.02808	0.39952
H125	0.31378	0.09948	0.49923
H126	0.29806	0.11153	0.57506
H127	0.41978	0.13738	0.61804
H128	0.43569	0.12593	0.54175
C129	0.38879	0.28032	0.03014
C130	0.42792	0.29165	0.04954
C131	0.43650	0.30320	0.09486
C132	0.40548	0.30511	0.12049
C133	0.36689	0.29590	0.10189
C134	0.35890	0.28307	0.05705
C135	0.47728	0.31219	0.11578
C136	0.49899	0.29207	0.10107
C137	0.53598	0.29925	0.12199
C138	0.55187	0.32596	0.15891
C139	0.53078	0.34658	0.17321
C140	0.49449	0.34028	0.15168
C141	0.33496	0.30018	0.12884
C142	0.34690	0.33291	0.15966
C143	0.31691	0.33827	0.18282
C144	0.27403	0.31114	0.17579
C145	0.26211	0.27787	0.14579
C146	0.29203	0.27241	0.12283
C147	0.37934	0.26588	0.98508
C148	0.33805	0.23708	0.97195
C149	0.32880	0.22128	0.92844
C150	0.36012	0.23451	0.89597
C151	0.40107	0.26399	0.90813
C152	0.41067	0.27897	0.95205
C153	0.35028	0.21614	0.85036
C154	0.58793	0.32979	0.18495
C155	0.24192	0.31835	0.19787
H156	0.45139	0.28994	0.02986
H157	0.41077	0.31271	0.15553
H158	0.32989	0.27748	0.04243
H159	0.48684	0.26959	0.07428
H160	0.55116	0.28246	0.11049
H161	0.54234	0.36761	0.20139
H162	0.47991	0.35748	0.16350
H163	0.37951	0.35525	0.16497
H164	0.32738	0.36433	0.20548

H165	0.22948	0.25610	0.13964
H166	0.28141	0.24632	0.10019
H167	0.31275	0.22470	0.99574
H168	0.29694	0.19844	0.92023
H169	0.42595	0.27482	0.88386
H170	0.44266	0.30194	0.95938
C171	0.71903	0.60993	0.46580
C172	0.71094	0.57238	0.44556
C173	0.69733	0.56343	0.40106
C174	0.69136	0.59265	0.37677
C175	0.69971	0.63086	0.39607
C176	0.71346	0.63890	0.44073
C177	0.69074	0.52410	0.37972
C178	0.72106	0.51201	0.38354
C179	0.71550	0.47561	0.36287
C180	0.67908	0.44980	0.33854
C181	0.64836	0.46148	0.33548
C182	0.65432	0.49838	0.35541
C183	0.69472	0.66269	0.36980
C184	0.66211	0.65079	0.33883
C185	0.65686	0.68084	0.31561
C186	0.68402	0.72370	0.32273
C187	0.71705	0.73555	0.35302
C188	0.72238	0.70560	0.37603
C189	0.73425	0.61930	0.51283
C190	0.76859	0.65817	0.52408
C191	0.78399	0.66658	0.56779
C192	0.76503	0.63663	0.60168
C193	0.73010	0.59803	0.59064
C194	0.71515	0.58934	0.54668
C195	0.78264	0.64526	0.64771
C196	0.67423	0.41235	0.31444
C197	0.67720	0.75597	0.30041
H198	0.71565	0.55015	0.46441
H199	0.68173	0.58623	0.34228
H200	0.71906	0.66750	0.45656
H201	0.74957	0.53127	0.40180
H202	0.73985	0.46772	0.36585
H203	0.62007	0.44255	0.31675
H204	0.63029	0.50669	0.35210
H205	0.63990	0.61817	0.33331
H206	0.63096	0.67043	0.29274
H207	0.73882	0.76817	0.35925
H208	0.74843	0.71622	0.39870
H209	0.78417	0.68179	0.49877

H210	0.81090	0.69664	0.57502
H211	0.71483	0.57419	0.61581
H212	0.68847	0.55921	0.53914
C213	0.89025	0.27670	0.46661
C214	0.86058	0.28466	0.44663
C215	0.86509	0.29847	0.40221
C216	0.90030	0.30475	0.37776
C217	0.93037	0.29657	0.39678
C218	0.92483	0.28262	0.44135
C219	0.83228	0.30503	0.38105
C220	0.78991	0.27456	0.38464
C221	0.75905	0.27997	0.36378
C222	0.76962	0.31641	0.33949
C223	0.81196	0.34731	0.33671
C224	0.84291	0.34149	0.35683
C225	0.96729	0.30213	0.37028
C226	0.98738	0.33477	0.33944
C227	0.02459	0.34040	0.31495
C228	0.04004	0.31324	0.32265
C229	0.01860	0.28042	0.35314
C230	0.98318	0.27494	0.37616
C231	0.88463	0.26128	0.51355
C232	0.88959	0.22712	0.52443
C233	0.88291	0.21155	0.56804
C234	0.87181	0.23016	0.60224
C235	0.86773	0.26491	0.59158
C236	0.87367	0.28003	0.54769
C237	0.86301	0.21218	0.64811
C238	0.73707	0.32110	0.31507
C239	0.07916	0.31982	0.30065
H240	0.83361	0.27969	0.46560
H241	0.90337	0.31453	0.34333
H242	0.94800	0.27715	0.45698
H243	0.78071	0.24602	0.40281
H244	0.72684	0.25549	0.36654
H245	0.82130	0.37561	0.31803
H246	0.87522	0.36563	0.35368
H247	0.97691	0.35696	0.33420
H248	0.04013	0.36628	0.29207
H249	0.02943	0.25868	0.35961
H250	0.96799	0.24883	0.39882
H251	0.89773	0.21181	0.49890
H252	0.88638	0.18478	0.57498
H253	0.85906	0.27989	0.61700
H254	0.86990	0.30658	0.54045

C255	0.10916	0.38519	0.96859
C256	0.13806	0.42370	0.94882
C257	0.13325	0.43348	0.90463
C258	0.09828	0.40461	0.87999
C259	0.06883	0.36590	0.89838
C260	0.07481	0.35669	0.94248
C261	0.16575	0.47322	0.88359
C262	0.20821	0.48527	0.88631
C263	0.23866	0.52152	0.86500
C264	0.22763	0.54724	0.84107
C265	0.18522	0.53569	0.83924
C266	0.15466	0.49895	0.85983
C267	0.03182	0.33477	0.87182
C268	0.01087	0.34740	0.84215
C269	0.97332	0.31626	0.81749
C270	0.95755	0.27336	0.82351
C271	0.97899	0.26084	0.85246
C272	0.01666	0.29185	0.87660
C273	0.11455	0.37520	0.01329
C274	0.09993	0.33350	0.02662
C275	0.10633	0.32380	0.07006
C276	0.12622	0.35513	0.10225
C277	0.13996	0.39653	0.08980
C278	0.13489	0.40652	0.04596
C279	0.13427	0.34499	0.14794
C280	0.25977	0.58442	0.81608
C281	0.91815	0.24154	0.80136
H282	0.16548	0.44584	0.96700
H283	0.09490	0.41176	0.84582
H284	0.05109	0.32790	0.95720
H285	0.21777	0.46599	0.90403
H286	0.27093	0.52931	0.86705
H287	0.17550	0.55453	0.82090
H288	0.12227	0.49065	0.85728
H289	0.02100	0.38009	0.83792
H290	0.95762	0.32726	0.79568
H291	0.96811	0.22812	0.85795
H292	0.03236	0.28059	0.89806
H293	0.08527	0.30813	0.00304
H294	0.09561	0.29160	0.07851
H295	0.15553	0.42143	0.11382
H296	0.14569	0.43888	0.03844
C297	0.89102	0.60439	0.02995
C298	0.86276	0.56577	0.04926
C299	0.86607	0.55724	0.09447

C300	0.89947	0.58822	0.11978
C301	0.92902	0.62665	0.10080
C302	0.92411	0.63428	0.05587
C303	0.83424	0.51667	0.11555
C304	0.79242	0.49507	0.10080
C305	0.76253	0.45821	0.12177
C306	0.77328	0.44237	0.15877
C307	0.81497	0.46333	0.17312
C308	0.84504	0.49950	0.15153
C309	0.96504	0.65889	0.12760
C310	0.98571	0.64738	0.15884
C311	0.02271	0.67937	0.18341
C312	0.03824	0.72203	0.17585
C313	0.01700	0.73352	0.14541
C314	0.97987	0.70159	0.12119
C315	0.88514	0.61437	0.98320
C316	0.88798	0.65278	0.97338
C317	0.88093	0.66200	0.93013
C318	0.87140	0.63330	0.89520
C319	0.86940	0.59516	0.90473
C320	0.87583	0.58565	0.94831
C321	0.86181	0.64272	0.84985
C322	0.74098	0.40654	0.18489
C323	0.07732	0.75442	0.19798
H324	0.83779	0.54267	0.02894
H325	0.90193	0.58313	0.15483
H326	0.94661	0.66339	0.04053
H327	0.78219	0.50722	0.07391
H328	0.73058	0.44310	0.11026
H329	0.82435	0.45177	0.20137
H330	0.87682	0.51400	0.16337
H331	0.97586	0.61489	0.16432
H332	0.03825	0.66913	0.20639
H333	0.02778	0.76603	0.13863
H334	0.96438	0.71198	0.09831
H335	0.89469	0.67542	0.99951
H336	0.88275	0.69166	0.92410
H337	0.86196	0.57228	0.87870
H338	0.87368	0.55590	0.95473
C339	0.27467	0.88973	0.96773
C340	0.28426	0.86103	0.94747
C341	0.29803	0.86575	0.90297
C342	0.30342	0.90057	0.87847
C343	0.29416	0.92988	0.89736
C344	0.27971	0.92387	0.94178

C345	0.30511	0.83321	0.88166
C346	0.27502	0.79070	0.88526
C347	0.28084	0.76009	0.86434
C348	0.31730	0.77100	0.83992
C349	0.34782	0.81349	0.83709
C350	0.34160	0.84420	0.85729
C351	0.29935	0.96685	0.87112
C352	0.33258	0.98815	0.84093
C353	0.33868	0.02391	0.81781
C354	0.31200	0.04038	0.82378
C355	0.27808	0.01947	0.85287
C356	0.27149	0.98179	0.87684
C357	0.25998	0.88424	0.01273
C358	0.23272	0.89838	0.02680
C359	0.21706	0.89160	0.07044
C360	0.22914	0.87181	0.10211
C361	0.25709	0.85866	0.08896
C362	0.27173	0.86412	0.04491
C363	0.21111	0.86312	0.14789
C364	0.32231	0.73856	0.81547
C365	0.32031	0.08002	0.80149
C366	0.97597	0.95366	0.25070
C367	0.02221	0.97627	0.25085
C368	0.11181	0.88411	0.25023
C369	0.28873	0.64210	0.24851
C370	0.30995	0.68606	0.24850
C371	0.28625	0.70930	0.24873
C372	0.30224	0.74806	0.27046
C373	0.28042	0.76995	0.27020
C374	0.24150	0.75341	0.24906
C375	0.21821	0.77659	0.24914
H376	0.27955	0.83376	0.96556
H377	0.31338	0.90392	0.84408
H378	0.27461	0.94744	0.95686
H379	0.24644	0.78117	0.90348
H380	0.25662	0.72778	0.86717
H381	0.37613	0.82311	0.81832
H382	0.36545	0.87662	0.85407
H383	0.35488	0.97779	0.83592
H384	0.36524	0.03936	0.79574
H385	0.25659	0.03075	0.85856
H386	0.24483	0.96606	0.89869
H387	0.22147	0.91286	0.00364
H388	0.19535	0.90188	0.07945
H389	0.26693	0.84321	0.11258

H390	0.29349	0.85372	0.03681
H391	0.95892	0.91992	0.25063
H392	0.25507	0.62508	0.24868
H393	0.33145	0.76143	0.28836
H394	0.29375	0.79962	0.28726
C395	0.04334	0.02006	0.25089
C396	0.02136	0.04203	0.25085
C397	0.11261	0.22396	0.25031
C398	0.35436	0.64254	0.24815
C399	0.31042	0.61981	0.24833
C400	0.28723	0.57290	0.24847
C401	0.24873	0.55008	0.27067
C402	0.22694	0.50638	0.27045
C403	0.24331	0.48405	0.24884
C404	0.22018	0.43760	0.24894
H405	0.07709	0.03722	0.25097
H406	0.37136	0.62588	0.24803
H407	0.23552	0.56590	0.28890
H408	0.19747	0.49001	0.28788
C409	0.61162	0.71921	0.96640
C410	0.57408	0.71175	0.94657
C411	0.56399	0.69692	0.90250
C412	0.59207	0.68913	0.87830
C413	0.63018	0.69675	0.89717
C414	0.63934	0.71170	0.94138
C415	0.52466	0.69074	0.88139
C416	0.51333	0.72168	0.88451
C417	0.47715	0.71657	0.86360
C418	0.45081	0.68000	0.83971
C419	0.46171	0.64868	0.83742
C420	0.49834	0.65416	0.85759
C421	0.66088	0.68996	0.87088
C422	0.64774	0.65660	0.84060
C423	0.67687	0.64985	0.81737
C424	0.71996	0.67616	0.82391
C425	0.73299	0.70991	0.85348
C426	0.70402	0.71676	0.87639
C427	0.62227	0.73544	0.01305
C428	0.66183	0.76929	0.02327
C429	0.67158	0.78531	0.06674
C430	0.64233	0.76739	0.10143
C431	0.60300	0.73300	0.09136
C432	0.59298	0.71751	0.04768
C433	0.65211	0.78559	0.14726
C434	0.41354	0.67544	0.81532

C435	0.75154	0.66829	0.80160
C436	0.97734	0.01979	0.25068
C437	0.95440	0.97587	0.25054
C438	0.77254	0.88568	0.24940
C439	0.35392	0.70773	0.24832
C440	0.37665	0.68650	0.24818
C441	0.42356	0.71018	0.24817
C442	0.44641	0.69432	0.27000
C443	0.49011	0.71617	0.26961
C444	0.51241	0.75497	0.24823
C445	0.55885	0.77835	0.24831
H446	0.55274	0.71781	0.96540
H447	0.58486	0.67863	0.84413
H448	0.66785	0.71673	0.95695
H449	0.53305	0.75035	0.90231
H450	0.46989	0.74140	0.86601
H451	0.44239	0.62024	0.81910
H452	0.50601	0.62964	0.85480
H453	0.61489	0.63504	0.83559
H454	0.66563	0.62351	0.79499
H455	0.76583	0.73119	0.85912
H456	0.71560	0.74339	0.89839
H457	0.68500	0.78397	-0.00266
H458	0.70212	0.81183	0.07318
H459	0.57962	0.71857	0.11712
H460	0.56234	0.69124	0.04098
H461	0.96074	0.03694	0.25057
H462	0.37060	0.74139	0.24832
H463	0.43062	0.66521	0.28808
H464	0.50651	0.70295	0.28678
C465	0.10534	0.71660	0.53192
C466	0.13376	0.70630	0.55108
C467	0.13015	0.69354	0.59606
C468	0.09624	0.69019	0.62124
C469	0.06651	0.69895	0.60244
C470	0.07183	0.71250	0.55782
C471	0.16201	0.68459	0.61702
C472	0.20389	0.70483	0.60241
C473	0.23372	0.69757	0.62321
C474	0.22290	0.67063	0.65995
C475	0.18117	0.64992	0.67418
C476	0.15116	0.65628	0.65274
C477	0.02974	0.69375	0.62908
C478	0.00910	0.66064	0.65952
C479	0.97344	0.65456	0.68259

C480	0.95720	0.68133	0.67591
C481	0.97836	0.71495	0.64627
C482	0.01404	0.72110	0.62333
C483	0.11106	0.73266	0.48512
C484	0.10751	0.76786	0.47523
C485	0.11395	0.78391	0.43181
C486	0.12346	0.76484	0.39675
C487	0.12630	0.72916	0.40645
C488	0.12054	0.71350	0.45013
C489	0.13210	0.78321	0.35096
C490	0.25516	0.66661	0.68583
C491	0.91752	0.67328	0.69794
C492	0.24736	0.69306	0.22722
C493	0.22515	0.71457	0.22779
H494	0.15900	0.70877	0.53078
H495	0.09344	0.68191	0.65609
H496	0.04920	0.71899	0.54259
H497	0.21424	0.72742	0.57574
H498	0.26569	0.71444	0.61176
H499	0.17168	0.62870	0.70220
H500	0.11936	0.63888	0.66449
H501	0.01977	0.63859	0.66462
H502	0.95804	0.62825	0.70497
H503	0.96711	0.73644	0.64036
H504	0.02934	0.74743	0.60099
H505	0.10061	0.78360	0.50140
H506	0.11156	0.81143	0.42572
H507	0.13380	0.71378	0.38040
H508	0.12322	0.68618	0.45650
H509	0.23415	0.66391	0.20922
H510	0.19542	0.70109	0.21085
C511	0.60955	0.88913	0.53125
C512	0.57057	0.86118	0.55027
C513	0.56144	0.86503	0.59522
C514	0.59233	0.89860	0.62051
C515	0.63109	0.92780	0.60184
C516	0.63921	0.92235	0.55724
C517	0.52032	0.83375	0.61610
C518	0.49799	0.79187	0.60155
C519	0.46070	0.76255	0.62245
C520	0.44504	0.77387	0.65920
C521	0.46670	0.81563	0.67330
C522	0.50329	0.84515	0.65178
C523	0.66321	0.96410	0.62854
C524	0.65165	0.98552	0.65896

C525	0.68156	0.02103	0.68219
C526	0.72462	0.03710	0.67609
C527	0.73728	0.01598	0.64687
C528	0.70591	0.97858	0.62273
C529	0.62002	0.88337	0.48453
C530	0.65874	0.88672	0.47491
C531	0.66876	0.88082	0.43147
C532	0.64061	0.87198	0.39613
C533	0.60207	0.86922	0.40558
C534	0.59178	0.87449	0.44926
C535	0.65080	0.86395	0.35029
C536	0.40865	0.74205	0.68533
C537	0.75622	0.07671	0.69819
C538	0.44612	0.74894	0.22639
C539	0.48984	0.77117	0.22682
H540	0.54761	0.83616	0.52990
H541	0.58691	0.90151	0.65535
H542	0.66853	0.94466	0.54212
H543	0.50985	0.78112	0.57488
H544	0.44509	0.73054	0.61107
H545	0.45536	0.82552	0.70132
H546	0.51821	0.87699	0.66346
H547	0.61906	0.97552	0.66399
H548	0.67073	0.03665	0.70435
H549	0.76998	0.02700	0.64103
H550	0.71653	0.96278	0.60059
H551	0.68109	0.89316	0.50128
H552	0.69866	0.88312	0.42560
H553	0.57953	0.86225	0.37929
H554	0.56184	0.87201	0.45542
H555	0.43010	0.76202	0.20831
H556	0.50602	0.80081	0.20969
C557	0.28068	0.38907	0.53134
C558	0.29089	0.42789	0.55023
C559	0.30412	0.43747	0.59506
C560	0.30790	0.40722	0.62036
C561	0.29919	0.36869	0.60183
C562	0.28533	0.36006	0.55735
C563	0.31308	0.47834	0.61588
C564	0.29249	0.49973	0.60159
C565	0.29963	0.53674	0.62254
C566	0.32681	0.55300	0.65907
C567	0.34793	0.53228	0.67290
C568	0.34169	0.49601	0.65132
C569	0.30447	0.33729	0.62866

C570	0.33769	0.34976	0.65899
C571	0.34368	0.32015	0.68217
C572	0.31669	0.27717	0.67562
C573	0.28299	0.26479	0.64611
C574	0.27692	0.29429	0.62316
C575	0.26424	0.37809	0.48471
C576	0.22921	0.33902	0.47538
C577	0.21310	0.32858	0.43203
C578	0.23193	0.35661	0.39649
C579	0.26738	0.39549	0.40566
C580	0.28309	0.40622	0.44926
C581	0.21354	0.34602	0.35072
C582	0.33077	0.58912	0.68522
C583	0.32419	0.24522	0.69766
C584	0.30330	0.55032	0.22647
C585	0.28188	0.50660	0.22705
H586	0.28800	0.45037	0.52985
H587	0.31641	0.41295	0.65514
H588	0.27894	0.33090	0.54232
H589	0.26971	0.48732	0.57511
H590	0.28248	0.55163	0.61138
H591	0.36936	0.54413	0.70072
H592	0.35939	0.48185	0.66279
H593	0.35985	0.38248	0.66392
H594	0.37003	0.33094	0.70448
H595	0.26128	0.23206	0.64039
H596	0.25045	0.28325	0.60100
H597	0.21372	0.31673	0.50191
H598	0.18575	0.29843	0.42637
H599	0.28256	0.41797	0.37923
H600	0.31027	0.43642	0.45519
H601	0.33225	0.56632	0.20812
H602	0.29520	0.49039	0.20973
Zn3	0.15697	0.29721	0.20188
Zn4	0.22223	0.36447	0.25829
Zn5	0.69908	0.85626	0.20129
Zn6	0.63182	0.85378	0.25803
Zn7	0.14058	0.83950	0.20200
Zn8	0.14285	0.77446	0.25881
Zn9	0.69866	0.84098	0.29670
Zn10	0.63215	0.77631	0.23931
Zn11	0.14248	0.29803	0.29739
Zn12	0.14491	0.36468	0.23995
Zn13	0.15596	0.85423	0.29742
Zn14	0.22041	0.85198	0.23977

Zn15	0.83609	0.68892	0.79819
Zn16	0.77276	0.62493	0.73945
Zn17	0.30194	0.14565	0.79697
Zn18	0.36708	0.14498	0.74057
Zn19	0.85436	0.15684	0.79760
Zn20	0.85289	0.22101	0.74023
Zn21	0.30313	0.16057	0.70136
Zn22	0.36897	0.22417	0.75826
Zn23	0.85229	0.69198	0.70275
Zn24	0.85139	0.62529	0.75745
Zn25	0.84017	0.14205	0.70213
Zn26	0.77506	0.14239	0.75832
Zn27	0.37526	0.71534	0.77164
Zn28	0.33746	0.62256	0.77147
Zn29	0.28247	0.66028	0.77191
Zn30	0.33147	0.66604	0.68925
Zn31	0.71387	0.37380	0.27110
Zn32	0.65908	0.28120	0.27126
Zn33	0.62128	0.33613	0.27109
Zn34	0.66458	0.33012	0.18878
O635	0.16662	0.33099	0.24938
O636	0.37207	0.23733	0.81717
O637	0.32002	0.17916	0.84526
O638	0.25288	0.34695	0.22715
O639	0.20392	0.29666	0.18583
O640	0.11746	0.24352	0.21383
O641	0.23945	0.41779	0.24145
O642	0.66546	0.83185	0.24883
O643	0.76167	0.13170	0.81711
O644	0.82072	0.14066	0.84577
O645	0.64887	0.90185	0.22689
O646	0.69920	0.90351	0.18538
O647	0.75293	0.87090	0.21298
O648	0.57852	0.81752	0.24148
O649	0.16493	0.83004	0.24949
O650	0.86261	0.62223	0.81608
O651	0.85270	0.67139	0.84559
O652	0.09501	0.74369	0.22741
O653	0.09335	0.79238	0.18589
O654	0.12616	0.87885	0.21373
O655	0.17898	0.75712	0.24262
O656	0.76051	0.62340	0.68041
O657	0.81987	0.67468	0.65371
O658	0.64899	0.74525	0.27073
O659	0.69887	0.79389	0.31266

O660	0.75258	0.88055	0.28566
O661	0.57869	0.75902	0.25525
O662	0.86348	0.23400	0.68123
O663	0.85509	0.17487	0.65353
O664	0.09682	0.34792	0.27090
O665	0.09529	0.29812	0.31322
O666	0.12776	0.24397	0.28647
O667	0.18114	0.41786	0.25652
O668	0.36932	0.13378	0.68177
O669	0.32012	0.14416	0.65322
O670	0.25161	0.89983	0.27114
O671	0.20323	0.90117	0.31347
O672	0.11688	0.86925	0.28647
O673	0.23766	0.81578	0.25573
O674	0.82814	0.65766	0.74940
O675	0.63062	0.76387	0.18037
O676	0.68169	0.82292	0.15263
O677	0.74086	0.64109	0.77081
O678	0.78917	0.68855	0.81478
O679	0.87349	0.74244	0.78817
O680	0.75669	0.57229	0.75535
O681	0.33533	0.16884	0.74937
O682	0.23277	0.86276	0.18076
O683	0.17395	0.85577	0.15342
O684	0.34896	0.09696	0.77218
O685	0.29946	0.09729	0.81331
O686	0.24951	0.13383	0.78473
O687	0.41985	0.18039	0.75724
O688	0.83057	0.16562	0.74959
O689	0.13471	0.36687	0.18097
O690	0.14105	0.31476	0.15325
O691	0.90091	0.25239	0.77155
O692	0.90147	0.20368	0.81380
O693	0.86930	0.11838	0.78609
O694	0.81631	0.23692	0.75688
O695	0.23509	0.36693	0.31725
O696	0.17618	0.31632	0.34578
O697	0.35250	0.25592	0.72721
O698	0.30277	0.20737	0.68530
O699	0.25017	0.12201	0.71256
O700	0.42116	0.23937	0.74106
O701	0.13180	0.76160	0.31771
O702	0.14006	0.82062	0.34579
O703	0.89948	0.64355	0.72592
O704	0.90125	0.69531	0.68713

O705	0.86205	0.74348	0.71603
O706	0.81548	0.57276	0.74020
O707	0.62959	0.86435	0.31699
O708	0.68053	0.85639	0.34512
O709	0.74475	0.09421	0.72707
O710	0.79432	0.09348	0.68648
O711	0.88128	0.13117	0.71397
O712	0.75821	0.17815	0.74129
O713	0.40803	0.74756	0.72706
O714	0.37946	0.70972	0.66643
O715	0.33167	0.66607	0.75092
O716	0.32718	0.61806	0.66637
O717	0.33703	0.58986	0.72693
O718	0.24983	0.66035	0.72758
O719	0.41095	0.70770	0.80653
O720	0.38541	0.63955	0.80230
O721	0.35830	0.74646	0.80259
O722	0.29015	0.70367	0.80657
O723	0.25178	0.61247	0.80332
O724	0.29446	0.58697	0.80658
O725	0.28762	0.67026	0.66676
O726	0.74629	0.40606	0.22665
O727	0.70849	0.37767	0.16596
O728	0.66470	0.33031	0.25039
O729	0.66841	0.28622	0.16615
O730	0.65916	0.24863	0.22695
O731	0.58857	0.33575	0.22671
O732	0.74479	0.35702	0.30229
O733	0.70236	0.28883	0.30598
O734	0.70641	0.40971	0.30553
O735	0.63824	0.38414	0.30179
O736	0.58580	0.29311	0.30614
O737	0.61140	0.25051	0.30248
O738	0.61686	0.32631	0.16599
C739	0.87447	0.76223	0.75320
C740	0.04541	0.95292	0.25085
C741	0.03624	0.92145	0.28240
C742	0.05819	0.89961	0.28266
C743	0.08900	0.90782	0.25050
C744	0.07662	0.96160	0.21912
C745	0.09773	0.93894	0.21856
H746	0.01242	0.91415	0.30730
H747	0.05060	0.87579	0.30762
H748	0.08420	0.98551	0.19426
H749	0.12135	0.94615	0.19344

C750	0.04458	0.08864	0.25087
C751	0.07468	0.11112	0.28365
C752	0.09626	0.15491	0.28387
C753	0.08911	0.17738	0.25061
C754	0.03695	0.11103	0.21800
C755	0.05930	0.15481	0.21753
H756	0.08112	0.09472	0.30947
H757	0.11904	0.17124	0.30976
H758	0.01407	0.09457	0.19224
H759	0.05288	0.17106	0.19152
C760	0.90781	0.95311	0.25007
C761	0.88532	0.96112	0.28249
C762	0.84152	0.93895	0.28261
C763	0.81910	0.90902	0.24960
C764	0.88545	0.92292	0.21735
C765	0.84168	0.90156	0.21675
H766	0.90170	0.98409	0.30819
H767	0.82516	0.94561	0.30827
H768	0.90192	0.91620	0.19186
H769	0.82546	0.87870	0.19091
Li70	1.04614	1.35705	1.07857
Li71	1.14929	1.36232	0.89501
Li72	1.18093	1.52192	0.96212
Li73	0.95316	1.30660	0.92000
Li74	1.42761	1.37299	1.05407
Li75	1.30700	1.25702	1.21770
Li76	1.46271	1.25570	1.19081
Li77	1.38594	1.19102	0.97104
Li78	1.21456	1.36326	1.59946
Li79	1.35570	1.31152	1.57922
Li80	1.29879	1.33518	1.43102
Li81	1.38139	1.55714	1.57672
Li82	0.93690	1.36971	1.44900
Li83	0.95233	1.25884	1.28161
Li84	0.79804	1.20583	1.50058
Li85	0.83403	1.27358	1.29523
Li86	0.99903	0.99782	1.33912
Li87	1.12428	1.12717	1.20054
Li88	0.89524	1.01014	1.19822
Li89	0.98882	0.88558	1.19625
Li90	1.33258	1.66390	1.33710
Li91	1.22481	1.52730	1.17394
Li92	1.30760	1.76803	1.17386
Li93	1.46085	1.68865	1.17331
Li94	0.78471	0.63734	0.39559

Li95	0.64269	0.68894	0.41751
Li96	0.69613	0.65805	0.56566
Li97	0.65495	0.47360	0.45636
Li98	0.77147	0.45496	0.82031
Li99	0.68403	0.22159	0.82148
Li0	0.66491	0.32845	0.65960
Li1	0.54080	0.31247	0.81954
Li2	1.14626	0.78320	0.59945
Li3	1.03308	0.69706	0.43463
Li4	0.95266	0.64192	0.57987
Li5	1.17151	0.61561	0.57824
Li6	0.56949	0.94195	0.55116
Li7	0.59353	0.78940	0.44850
Li8	0.53317	0.79092	0.69164
Li9	0.68835	0.94678	0.71671
Li10	0.31022	1.04747	0.28411
Li11	0.43248	1.05949	0.45086
Li12	0.40257	1.20311	0.53115
Li13	0.46810	1.18598	0.27996
Li14	0.68561	0.63714	0.91952
Li15	0.66048	0.69598	1.06384
Li16	0.63994	0.78296	0.89398
Li17	0.45354	0.65302	0.94208
C818	0.95264	0.97801	0.75149
C819	0.97509	0.95422	0.75156
H820	0.91891	0.96143	0.75182
C821	1.01889	0.97674	0.75108
C822	1.04100	1.02069	0.75061
H823	1.03593	0.96003	0.75108
C824	1.01891	1.04262	0.75052
C825	0.97499	1.02178	0.75090
H826	1.03617	1.07637	0.75009
C827	0.95159	0.90768	0.75202
C828	0.92042	0.88574	0.78396
C829	0.89844	0.84195	0.78465
C830	0.90620	0.81900	0.75254
C831	0.95983	0.88479	0.72032
C832	0.93702	0.84101	0.72019
H833	0.91347	0.90254	0.80884
H834	0.87486	0.82601	0.80991
H835	0.98350	0.90084	0.69516
H836	0.94388	0.82433	0.69510
C837	1.08761	1.04391	0.75007
C838	1.11034	1.03646	0.78268
C839	1.15414	1.05853	0.78239

C840	1.17634	1.08782	0.74877
C841	1.10974	1.07362	0.71685
C842	1.15351	1.09490	0.71586
H843	1.09415	1.01387	0.80877
H844	1.17067	1.05221	0.80816
H845	1.09308	1.07991	0.69120
H846	1.16956	1.11732	0.68959
C847	0.95239	1.04576	0.75052
C848	0.96085	1.07656	0.78270
C849	0.93883	1.09835	0.78291
C850	0.90859	1.09068	0.75022
C851	0.92189	1.03777	0.71811
C852	0.90068	1.06032	0.71759
H853	0.98406	1.08329	0.80816
H854	0.94585	1.12162	0.80839
H855	0.91482	1.01434	0.69281
H856	0.87757	1.05355	0.69200
Li57	1.00814	0.89662	0.80619
Li58	1.10388	1.11572	0.80007
Li59	0.88114	0.99197	0.80234
Li60	0.99600	0.99808	0.66255
Li61	0.78275	1.14688	1.09778
Li62	0.61386	1.17019	1.07767
Li63	0.64384	0.95329	1.07939
Li64	0.70711	1.03195	0.91408
Li65	0.21051	0.84891	0.89534
Li66	0.35001	1.04449	0.92033
Li67	0.34545	0.79236	0.94137
Li68	0.31185	0.95366	1.07422
Li69	0.84887	0.63030	1.09527
Li70	0.82474	0.43803	1.07748
Li71	0.96242	0.65756	0.93123
Li72	1.04447	0.68638	1.08144

8.5 MOF200-Li

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Name
MOF200-Li

Space group symmetry
P 1

 a    b    c
 51.4517  51.4517 41.7962 A

 alpha   betha   gamma
 90.000  90.000  120.000
```

Atom	x	y	z
C1	14.632301331	35.067665100	11.918254852
O1	13.746623039	34.719009399	11.073466301
C2	1.384109974	23.947683334	27.004907608
C3	3.601633072	24.483877182	27.803308487
C4	2.731891870	14.753588676	17.020256042
C5	3.379968643	16.982566833	16.344593048
C6	8.657975197	11.154540062	27.519468307
C7	9.545258522	12.842576981	29.002607346
C8	4.668336868	18.689945221	24.747247696
C9	4.335594654	18.388339996	23.418119431
C10	4.708024025	17.171703339	22.833734512
C11	5.412717342	16.239919662	23.606210709
C12	5.772374153	16.514657974	24.935981750
C13	5.399247169	17.750284195	25.496978760
C14	4.355494976	16.873947144	21.426206589
C15	4.062971592	17.912843704	20.528972626
C16	3.726485968	17.633277893	19.201141357
C17	3.665382624	16.307518005	18.744979858
C18	3.956812620	15.268260956	19.642299652
C19	4.305380344	15.548874855	20.967098236
C20	6.516613960	15.497603416	25.723264694
C21	6.643351555	14.187852859	25.234508514
C22	7.345907688	13.220035553	25.954137802
C23	7.948111534	13.534569740	27.181535721
C24	7.823518276	14.844746590	27.675445557
C25	7.111197472	15.815427780	26.956027985
C26	4.202766895	19.962480545	25.348371506
C27	4.867990017	20.538509369	26.441768646
C28	4.406427383	21.737449646	27.001928329

C29	3.263735056	22.374074936	26.488655090
C30	2.598506212	21.793487549	25.399631500
C31	3.067045689	20.606519699	24.832117081
C32	2.746795416	23.621082306	27.100185394
C33	3.265357018	16.008657455	17.350154877
C34	8.718294144	12.499563217	27.919519424
C35	10.306485176	11.863944054	29.656719208
C36	9.411839485	10.178050041	28.175451279
C37	2.302695513	14.484506607	15.718537331
C38	2.962188005	16.708587646	15.037302017
C39	2.412804127	15.459280014	14.717108727
C40	10.247767448	10.523438454	29.244880676
C41	0.881854117	25.100307465	27.618337631
C42	3.101826906	25.644918442	28.404045105
C43	1.737430930	25.958913803	28.321895599
C44	1.199083567	27.127031326	29.046890259
C45	1.890456080	15.191305161	13.365027428
O2	-0.038104441	27.164403915	29.335941315
O3	1.990471363	28.050170898	29.414424896
O4	10.932445526	8.163168907	29.483245850
O5	2.245920658	15.930008888	12.390657425
O6	1.082160711	14.224075317	13.201244354
C46	26.911809921	15.586227417	31.210142136
C47	25.683074951	16.263439178	31.210079193
C48	28.274389267	13.481937408	31.212989807
C49	28.332378387	12.083334923	31.113159180
C50	30.704767227	13.537558556	31.325452805
C51	30.762229919	12.138922691	31.224533081
C52	32.065814972	11.432681084	31.235576630
C53	33.261569977	12.137217522	31.451786041
C54	34.488834381	11.467948914	31.471334457
C55	34.543167114	10.082180023	31.271408081
C56	35.833457947	9.371053696	31.303062439
O7	35.867916107	8.124215126	31.056612015
O8	25.029912949	32.516685486	30.468412399
C57	25.398689270	33.108470917	31.531198502
C58	25.424531937	34.576389313	31.575122833
C59	26.174592972	35.240615845	32.554111481
C60	26.213361740	36.636184692	32.584487915
C61	25.490968704	37.387668610	31.645856857
C62	25.532979965	38.862518311	31.675745010
C63	24.470939636	39.614727020	31.152971268
C64	24.512504578	41.009918213	31.179311752
C65	25.622932434	41.677742004	31.715520859
C66	25.675273895	43.152000427	31.726476669

C67	24.493526459	43.904937744	31.725957870
O9	-13.059262276	36.842285156	10.380498886
O10	0.000000000	29.705627441	30.972063065
ZN1	0.558911622	13.787817001	8.924454689
ZN2	23.958002090	28.656476974	31.145679474
ZN3	-0.724388957	31.267477036	30.359127045
ZN4	0.000000000	29.705627441	32.808902740
C68	-11.959812164	39.696556091	11.918254852
O11	-11.215025902	39.103862762	11.073466301
C69	4.294471264	33.783275604	27.004907608
C70	2.721351624	35.435607910	27.803308487
C71	11.582900047	39.547534943	17.020256042
C72	9.328509331	38.994297028	16.344593048
C73	37.462554932	1.920756340	27.519468307
C74	35.557029724	1.845148087	29.002607346
C75	7.205693722	39.256366730	24.747247696
C76	7.633261681	39.119007111	23.418119431
C77	8.500685692	40.049858093	22.833734512
C78	8.955287933	41.126033783	23.606210709
C79	8.537528992	41.300136566	24.935981750
C80	7.654007912	40.359184265	25.496978760
C81	8.934814453	39.893436432	21.426206589
C82	8.181365013	39.120658875	20.528972626
C83	8.591719627	38.969036102	19.201141357
C84	9.770412445	39.578998566	18.744979858
C85	10.524720192	40.351013184	19.642299652
C86	10.107418060	40.512573242	20.967098236
C87	9.046203613	42.453193665	25.723264694
C88	10.117111206	43.217826843	25.234508514
C89	10.603988647	44.310165405	25.954137802
C90	35.756320953	0.115981795	27.181535721
C91	8.958141327	43.911434174	27.675445557
C92	8.473667145	42.809204102	26.956027985
C93	6.336429119	38.216903687	25.348371506
C94	5.504962921	38.504989624	26.441768646
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C96	4.717443466	36.197883606	26.488655090
C97	5.552862644	35.912071228	25.399631500
C98	6.346536160	36.911323547	24.832117081
C99	3.895972967	35.126693726	27.100185394
C100	10.229246140	39.381996155	17.350154877
C101	36.267570496	1.300482392	27.919519424
C102	36.023937225	2.993705988	29.656719208
C103	37.931285858	3.061866760	28.175451279
C104	12.030529976	39.310382843	15.718537331

C105	9.774673462	38.769477844	15.037302017
C106	11.131298065	38.918350220	14.717108727
C107	37.214210510	3.613107920	29.244880676
C108	3.547397614	32.771995544	27.618337631
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C110	2.376034021	33.083644867	28.321895599
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C112	11.624544144	38.599971771	13.365027428
O12	2.219816446	30.943241119	29.335941315
O13	0.438432157	32.257156372	29.414424896
O14	38.915924072	5.386190891	29.483245850
O15	10.807076454	38.538463593	12.390657425
O16	12.866337776	38.383583069	13.201244354
C113	24.497682571	15.513197899	31.210142136
C114	24.525568008	14.110476494	31.210079193
C115	25.638761520	17.745370865	31.212989807
C116	26.820993423	18.494892120	31.113159180
C117	24.375404358	19.822328568	31.325452805
C118	25.557926178	20.571411133	31.224533081
C119	25.517757416	22.053468704	31.235576630
C120	24.309732437	22.736757278	31.451786041
C121	24.275705338	24.134231567	31.471334457
C122	25.448650360	24.874168396	31.271408081
C123	25.419357300	26.347156525	31.303062439
O17	26.481922150	27.000417709	31.056612015
O18	10.776426315	5.418197632	30.468412399
C124	10.079534531	5.441673756	31.531198502
C125	8.795360565	4.730095387	31.575122833
C126	7.845090866	5.047554493	32.554111481
C127	6.617108822	4.383344173	32.584487915
C128	6.327500820	3.381992102	31.645856857
C129	5.029239655	2.680950403	31.675745010
C130	4.908827305	1.385090709	31.152971268
C131	3.679774046	0.723492444	31.179311752
C132	2.546206713	1.351238132	31.715520859
C133	1.243293405	0.659439802	31.726476669
C134	-24.543725967	43.817989349	31.725957870
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C138	-14.314792633	34.815761566	17.020256042
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C146	-14.309903145	31.302091599	24.935981750
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C152	-14.481533051	33.497612000	19.642299652
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C155	-16.760463715	31.711204529	25.234508514
C156	-17.949895859	31.586681366	25.954137802
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C158	-16.781660080	30.360702515	27.675445557
C159	-15.584864616	30.492250443	26.956027985
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C168	32.191619873	30.758396149	27.919519424
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C170	29.834358215	31.318525314	28.175451279
C171	-14.333225250	35.321994781	15.718537331
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O21	-2.181711912	31.009239197	29.335941315
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O23	27.329118729	31.009082794	29.483245850

O24	-13.052996635	34.648414612	12.390657425
O25	-13.948497772	36.509223938	13.201244354
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C181	26.968841553	14.184527397	31.210079193
C182	23.264333725	13.331133842	31.212989807
C183	22.024114609	13.980215073	31.113159180
C184	22.097314835	11.198554039	31.325452805
C185	20.857328415	11.848107338	31.224533081
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C187	19.606182098	9.684468269	31.451786041
C188	18.412946701	8.956261635	31.471334457
C189	17.185668945	9.602093697	31.271408081
C190	15.924671173	8.840230942	31.303062439
O26	14.827648163	9.433808327	31.056612015
O27	41.371147156	6.623559952	30.468412399
C191	41.699260712	6.008296490	31.531198502
C192	42.957595825	5.251957893	31.575122833
C193	43.157802582	4.270270348	32.554111481
C194	44.347015381	3.538912296	32.584487915
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C197	47.797718048	3.558623791	31.152971268
C198	48.985206604	2.825031757	31.179311752
C199	49.008346558	1.529460549	31.715520859
C200	50.258918762	0.747003734	31.726476669
C201	0.050199650	1.393956661	31.725957870
O28	12.710157394	37.446952820	10.380498886
ZN8	-14.064684868	37.180503845	8.924454689
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C202	3.352558374	14.481327057	8.815986633
O29	3.199261189	15.396826744	9.687789917
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C205	13.543465614	35.195701599	3.746890545
C206	12.061456680	33.492862701	4.614428520
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C208	18.748828888	29.615650177	33.956707001
C209	11.297001839	30.753656387	38.173675537
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C212	13.724347115	31.552160263	39.324516296
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C219	13.710920334	33.679080963	1.254409909
C220	13.655884743	33.108741760	41.779449463
C221	14.979974747	30.867031097	37.270133972
C222	16.161190033	31.463890076	37.733058929
C223	17.345159531	31.348770142	37.004230499
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C231	7.587872505	30.405168533	37.432807922
C232	8.783096313	30.640155792	38.123874664
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O32	23.413644791	30.915239334	33.372451782
O33	12.606396675	35.205818176	8.442334175
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C250	33.352863312	9.375753403	31.051843643
O35	36.899463654	10.006446838	31.583604813
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O40	40.792388916	8.824011803	33.372451782
O41	-1.539894819	16.038074493	8.442334175
O42	-0.333125204	14.425727844	7.509269238
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O43	15.941934586	7.599346161	31.583604813
O44	25.747297287	32.440555573	32.554935455
C304	24.706283569	35.323726654	30.633022308
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O48	12.971452713	4.819191933	33.372451782
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O50	-13.066219330	37.634075165	7.509269238
C353	24.415117264	18.425273895	31.318141937
C354	26.781013489	19.891351700	31.117509842
C355	26.689767838	22.800403595	31.035316467
C356	26.655584335	24.196550369	31.051843643
O51	24.336088181	26.952650070	31.583604813
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C369	21.390233994	26.170103073	18.378042221
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C376	21.999341965	26.925165176	22.595020294
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C378	21.769016266	29.290182114	22.153862000
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O54	25.763933182	17.394037247	12.460219383
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O93	27.265724182	28.520368576	33.353828430
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C661	4.891092777	31.311080933	10.678651810
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C663	8.556790352	33.572303772	10.744318962
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8.6 MOF210-Li

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Name
MOF210-Li

Space group symmetry
R -3

 a   b  c
 50.745  50.745 194.256  A

 alpha   betha  gamma
 90.000  90.000 120.000
```

Atom	x	y	z
Zn1	0.72200	0.59200	0.19630
Zn2	0.69200	0.62300	0.18770
Zn3	0.69500	0.62800	0.20390
Zn4	0.65100	0.56500	0.19690
Zn5	0.69900	0.58800	0.08140
Zn6	0.65800	0.61000	0.07600
Zn7	0.63300	0.55500	0.08530
Zn8	0.67500	0.61700	0.09100
Zn9	0.62300	0.69300	0.31200
Zn10	0.59300	0.72100	0.30360
Zn11	0.56700	0.65200	0.30330
Zn12	0.62800	0.69500	0.29640
O13	0.69010	0.60180	0.19620
O14	0.66620	0.59250	0.08340
O15	0.60290	0.69030	0.30380
O16	0.74700	0.61000	0.20360
O17	0.62900	0.56100	0.18940
O18	0.65900	0.60200	0.18300
O19	0.73000	0.63700	0.20880
O20	0.63200	0.56600	0.20440
O21	0.74500	0.60600	0.18870
O22	0.70700	0.55200	0.19690
O23	0.65600	0.53300	0.19740
O24	0.32500	0.29600	0.14380
O25	0.64800	0.60000	0.09740
O26	0.61800	0.55400	0.09340
O27	0.31800	0.31000	0.24470
O28	0.31100	0.31800	0.25560
O29	0.95500	0.70500	0.23890

O30	0.93600	0.72600	0.24590
O31	0.25100	0.29700	0.26130
O32	0.21100	0.27500	0.25440
O33	0.99300	0.72400	0.34960
O34	0.96300	0.73400	0.35580
O35	0.53400	0.65600	0.30260
O36	0.32900	0.29800	0.13240
O37	0.66400	0.61000	0.20940
O38	0.56700	0.63100	0.29600
O39	0.61100	0.66300	0.29080
O40	0.66300	0.69900	0.29910
O41	0.98300	0.71500	0.26440
O42	0.95200	0.73100	0.26050
O43	0.65900	0.69700	0.31050
O44	0.97600	0.78400	0.25190
O45	1.02500	0.80800	0.24870
O46	0.55300	0.70600	0.30310
O47	0.13700	0.39000	0.29630
O48	0.09200	0.36300	0.29110
O49	0.72400	0.62900	0.18280
O50	1.07900	0.80500	0.35550
O51	1.05800	0.76200	0.34960
C52	0.74900	0.62800	0.20830
C53	0.74500	0.62200	0.18360
C54	0.68000	0.53000	0.19740
C55	0.60900	0.56600	0.10470
C56	0.32700	0.32600	0.25010
C57	0.93400	0.71000	0.24050
C58	0.67400	0.69800	0.30500
C59	0.96800	0.72300	0.35040
C60	0.53000	0.67900	0.30260
C61	0.63400	0.57700	0.18390
C62	0.61100	0.56800	0.17840
C63	0.57000	0.52800	0.17180
H64	0.55430	0.50740	0.17120
C65	0.58800	0.53700	0.17760
H66	0.58550	0.52260	0.18110
C67	0.53200	0.52100	0.14820
C68	0.54700	0.53600	0.14220
H69	0.56590	0.55470	0.14240
C70	0.53500	0.52300	0.13570
C71	0.50700	0.49600	0.13540
H72	0.49890	0.48700	0.13100
C73	0.49200	0.48100	0.14140
C74	0.50400	0.49400	0.14780

H75	0.49390	0.48360	0.15190
C76	0.42000	0.39600	0.14000
C77	0.40500	0.38000	0.14600
H78	0.41280	0.38820	0.15040
C79	0.38000	0.35100	0.14540
H80	0.36990	0.33960	0.14950
C81	0.36800	0.33800	0.13890
C82	0.38400	0.35400	0.13300
H83	0.37640	0.34540	0.12850
C84	0.40900	0.38300	0.13350
H85	0.41930	0.39410	0.12950
C86	0.33900	0.30900	0.13800
C87	0.57900	0.55200	0.11740
C88	0.61800	0.58800	0.10990
H89	0.63400	0.60830	0.10910
C90	0.60300	0.58100	0.11620
H91	0.60890	0.59630	0.11970
C92	0.61300	0.58900	0.17350
H93	0.62800	0.61020	0.17420
C94	0.59500	0.58000	0.16770
H95	0.59670	0.59490	0.16440
C96	0.57300	0.55000	0.16680
C97	0.55100	0.53600	0.12950
C98	0.56400	0.54400	0.12400
C99	0.44500	0.42600	0.14060
C100	0.46600	0.45100	0.14100
C101	0.55800	0.54000	0.16030
C102	0.54600	0.53200	0.15480
C103	0.56900	0.53000	0.11230
H104	0.55240	0.50990	0.11310
C105	0.58400	0.53700	0.10590
H106	0.57750	0.52170	0.10240
C107	0.63900	0.58500	0.20930
C108	0.61800	0.57700	0.21510
C109	0.57300	0.53900	0.22120
H110	0.55480	0.51990	0.22130
C111	0.59100	0.54900	0.21530
H112	0.58460	0.53580	0.21140
C113	0.53900	0.52200	0.24510
C114	0.55200	0.53700	0.25130
H115	0.57050	0.55580	0.25130
C116	0.53700	0.52400	0.25750
C117	0.51000	0.49600	0.25740
H118	0.49980	0.48690	0.26160
C119	0.49700	0.48200	0.25120

C120	0.51200	0.49500	0.24500
H121	0.50350	0.48470	0.24070
C122	0.41500	0.40500	0.25070
C123	0.40400	0.38900	0.24460
H124	0.41690	0.39490	0.24060
C125	0.37500	0.36300	0.24440
H126	0.36840	0.35150	0.24020
C127	0.35700	0.35400	0.25020
C128	0.36700	0.37100	0.25630
H129	0.35490	0.36500	0.26030
C130	0.39600	0.39700	0.25650
H131	0.40340	0.40830	0.26060
C132	0.56600	0.57300	0.27490
C133	0.60100	0.62100	0.28030
H134	0.61990	0.63940	0.28040
C135	0.59400	0.60000	0.27500
H136	0.60780	0.60480	0.27130
C137	0.62600	0.59600	0.22090
H138	0.64310	0.61610	0.22070
C139	0.60800	0.58700	0.22680
H140	0.61320	0.60000	0.23070
C141	0.58200	0.55800	0.22700
C142	0.54800	0.54000	0.26380
C143	0.55700	0.55500	0.26900
C144	0.44400	0.43200	0.25090
C145	0.46900	0.45400	0.25100
C146	0.56600	0.54600	0.23340
C147	0.55400	0.53600	0.23870
C148	0.54500	0.56600	0.28030
H149	0.52650	0.54770	0.28040
C150	0.55200	0.58700	0.28580
H151	0.53840	0.58220	0.28950
C152	0.58000	0.61500	0.28570
C153	0.58600	0.63700	0.29120
C154	0.96000	0.71900	0.26520
C155	0.94300	0.70900	0.27170
C156	0.90200	0.70400	0.27910
H157	0.88490	0.70660	0.27990
C158	0.91700	0.71300	0.27290
H159	0.91070	0.72100	0.26930
C160	0.86700	0.67600	0.30250
C161	0.87900	0.67500	0.30890
H162	0.89770	0.67480	0.30920
C163	0.86400	0.67600	0.31500
C164	0.83700	0.67600	0.31460

H165	0.82680	0.67620	0.31870
C166	0.82500	0.67700	0.30820
C167	0.84000	0.67700	0.30210
H168	0.83160	0.67710	0.29780
C169	0.75400	0.69100	0.30670
C170	0.74300	0.69300	0.30020
H171	0.75310	0.69230	0.29610
C172	0.71800	0.69700	0.29960
H173	0.71040	0.69840	0.29520
C174	0.70300	0.69900	0.30560
C175	0.71400	0.69800	0.31210
H176	0.70480	0.69950	0.31610
C177	0.74000	0.69400	0.31260
H178	0.74750	0.69350	0.31700
C179	0.90700	0.69000	0.33340
C180	0.94900	0.69200	0.33980
H181	0.96440	0.68680	0.34030
C182	0.93000	0.68200	0.33410
H183	0.93230	0.66990	0.33070
C184	0.95200	0.69600	0.27690
H185	0.96890	0.69320	0.27620
C186	0.93700	0.68800	0.28320
H187	0.94300	0.67900	0.28670
C188	0.91200	0.69200	0.28430
C189	0.87800	0.67900	0.32150
C190	0.89100	0.68300	0.32700
C191	0.77900	0.68600	0.30730
C192	0.80000	0.68200	0.30770
C193	0.89700	0.68500	0.29090
C194	0.88400	0.68000	0.29630
C195	0.90300	0.70600	0.33850
H196	0.88660	0.71080	0.33810
C197	0.92200	0.71600	0.34430
H198	0.91850	0.72740	0.34780
C199	0.94600	0.71000	0.34490
C200	1.00000	0.83700	0.25040
C201	0.97400	0.86600	0.25230
H202	0.95610	0.86590	0.25350
C203	0.97400	0.83800	0.25230
H204	0.95600	0.81970	0.25340
C205	1.00000	0.97300	0.25080
C206	1.02800	1.00000	0.25080
H207	1.04640	1.00030	0.25080
C208	1.00000	0.89300	0.25060
C209	1.02700	0.86500	0.24870

H210	1.04500	0.86440	0.24750
C211	1.02700	0.89200	0.24880
H212	1.04490	0.91060	0.24770
C213	1.00000	0.94400	0.25070
C214	1.00000	0.92100	0.25070
C215	1.00000	0.80800	0.25030
C216	0.67600	0.49900	0.19800
C217	0.69800	0.46700	0.19890
H218	0.71570	0.46460	0.19900
C219	0.70200	0.49600	0.19810
H220	0.72130	0.51290	0.19760
C221	0.66600	0.36100	0.20140
C222	0.63900	0.33300	0.20140
H223	0.61990	0.33240	0.20140
C224	0.64700	0.47400	0.19870
H225	0.62920	0.47570	0.19860
C226	0.66900	0.44200	0.19960
C227	0.64300	0.44500	0.19950
H228	0.62370	0.42730	0.19990
C229	0.66600	0.38800	0.20100
C230	0.66700	0.41200	0.20040
C231	0.36000	0.66600	0.29970
C232	0.36100	0.69400	0.29970
H233	0.38030	0.71220	0.29960
C234	0.44100	0.66900	0.30080
C235	0.46700	0.69800	0.30120
H236	0.46480	0.71500	0.30110
C237	0.49600	0.70100	0.30180
H238	0.51320	0.72070	0.30210
C239	0.50000	0.67500	0.30200
C240	0.47400	0.64600	0.30160
H241	0.47590	0.62850	0.30170
C242	0.44500	0.64300	0.30100
H243	0.42720	0.62300	0.30070
C244	0.38800	0.66500	0.29990
C245	0.41200	0.66600	0.30030
C246	0.81900	0.63700	0.21820
H247	0.83060	0.62790	0.21830
C248	0.79400	0.62700	0.21360
H249	0.78940	0.60990	0.21070
C250	0.77500	0.64000	0.21340
C251	0.78200	0.66400	0.21780
H252	0.76960	0.67330	0.21780
C253	0.80700	0.67500	0.22240
H254	0.81140	0.69200	0.22530

C255	0.82600	0.66200	0.22260
C256	0.88000	0.67300	0.22530
H257	0.88000	0.66470	0.22100
C258	0.85400	0.67500	0.22720
C259	0.85400	0.68800	0.23370
H260	0.83720	0.68940	0.23510
C261	0.88000	0.69900	0.23800
H262	0.88010	0.70840	0.24230
C263	0.90600	0.69800	0.23600
C264	0.90500	0.68400	0.22960
H265	0.92240	0.68300	0.22820
C266	0.22200	0.31800	0.27040
H267	0.24060	0.31990	0.27190
C268	0.20900	0.30400	0.26410
C269	0.18200	0.30200	0.26210
H270	0.17270	0.29300	0.25780
C271	0.16700	0.31400	0.26630
H272	0.14860	0.31210	0.26480
C273	0.18000	0.32700	0.27270
C274	0.18100	0.36500	0.28160
H275	0.20290	0.37470	0.28150
C276	0.16400	0.33900	0.27730
C277	0.13200	0.32600	0.27760
H278	0.12000	0.30890	0.27470
C279	0.11800	0.33700	0.28210
H280	0.09640	0.32720	0.28210
C281	0.13500	0.36100	0.28650
C282	0.16700	0.37500	0.28620
H283	0.17930	0.39230	0.28900
C284	0.12100	0.37200	0.29160
C285	0.22500	0.29200	0.25970
C286	0.81900	0.64200	0.17480
H287	0.83590	0.63840	0.17550
C288	0.79500	0.62900	0.17940
H289	0.79480	0.61700	0.18310
C290	0.77000	0.63300	0.17840
C291	0.77000	0.65000	0.17270
H292	0.75250	0.65250	0.17190
C293	0.79400	0.66300	0.16810
H294	0.79330	0.67380	0.16430
C295	0.82000	0.65900	0.16910
C296	1.12700	0.79800	0.33480
H297	1.12620	0.78650	0.33090
C298	1.10300	0.78700	0.33940
H299	1.08570	0.76710	0.33860

C300	1.10300	0.80300	0.34520
C301	1.12800	0.83300	0.34620
H302	1.12890	0.84440	0.35000
C303	1.15300	0.84400	0.34150
H304	1.16980	0.86410	0.34230
C305	1.15300	0.82700	0.33580
C306	1.07900	0.79000	0.35030
C307	0.62600	0.57300	0.09810
C308	0.20700	0.32900	0.27470
H309	0.21610	0.33810	0.27900
Li10	0.54721	0.62009	0.27318
Li11	0.49398	0.53980	0.25053
Li12	0.56768	0.59293	0.21621
Li13	0.36268	0.41510	0.24649
Li14	0.48967	0.53985	0.14151
Li15	0.55105	0.56785	0.17958
Li16	0.35834	0.39179	0.13909
Li17	0.55543	0.57686	0.10619
Li18	0.83859	0.69012	0.20860
Li19	0.90170	0.74045	0.22550
Li20	0.66892	0.46375	0.18503
Li21	0.96436	0.75650	0.28292
Li22	0.88385	0.73710	0.30865
Li23	0.76597	0.75593	0.30605
Li24	0.96496	0.75066	0.33246
Li25	0.47608	0.67353	0.28767
Li26	0.22516	0.37094	0.26254
Li27	0.15161	0.38757	0.27174
Li28	1.09934	0.83917	0.33323
Li29	0.98268	0.85644	0.23728
Li30	0.76555	0.59372	0.16642
Li31	0.33333	0.66667	0.31333
Li32	1.00000	1.00000	0.23688
Li33	0.66667	0.33333	0.21529

8.7 MOF180-Li

```
Name
MOF180-Li

Space group symmetry
P 1

 a       b       c
 45.846  45.846  37.110A

 alpha   betha  gamma
 90.000  90.000 120.000
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Atom	x	y	z
Zn1	0.15630	0.30302	0.21060
Zn2	0.14869	0.36437	0.24100
O3	0.16765	0.33530	0.25000
O4	0.14150	0.36250	0.19640
O5	0.14830	0.32160	0.17410
O6	0.89000	0.19590	0.79950
O7	0.88850	0.23520	0.76650
O8	0.12760	0.26560	0.22110
O9	0.17760	0.40210	0.25640
C10	0.10830	0.38900	0.95730
C11	0.08030	0.36560	0.93720
C12	0.07590	0.37250	0.90130
C13	0.09990	0.40310	0.88550
C14	0.12800	0.42670	0.90530
C15	0.13210	0.41950	0.94120
C16	0.11300	0.38150	0.99420
C17	0.11730	0.37530	0.02490
C18	0.12280	0.36750	0.06140
C19	0.12210	0.38640	0.09080
C20	0.12790	0.37910	0.12600
C21	0.13480	0.35280	0.13240
C22	0.13530	0.33380	0.10270
C23	0.12940	0.34120	0.06760
C24	0.14190	0.34530	0.16970
C25	0.04690	0.34800	0.88070
C26	0.02260	0.32720	0.86380
C27	0.99330	0.30200	0.84410
C28	0.97970	0.26770	0.85210
C29	0.95080	0.24330	0.83400

C30	0.93490	0.25260	0.80750
C31	0.94910	0.28710	0.79930
C32	0.97800	0.31150	0.81740
C33	0.90290	0.22650	0.78980
C34	0.15310	0.45810	0.88870
C35	0.17410	0.48420	0.87470
C36	0.12485	0.24970	0.25000
C37	0.10600	0.21200	0.25000
C38	0.10240	0.19340	0.28240
C39	0.08440	0.15850	0.27940
C40	0.06965	0.13930	0.25000
C41	0.05140	0.10280	0.25000
C42	0.03610	0.07220	0.25000
C43	0.01775	0.03550	0.25000
C44	0.03530	0.01765	0.25000
C45	0.20900	0.41800	0.25000
C46	0.22790	0.45580	0.25000
C47	0.21120	0.47400	0.25690
C48	0.22890	0.50940	0.25690
C49	0.26365	0.52730	0.25000
C50	0.28195	0.56390	0.25000
C51	0.29725	0.59450	0.25000
C52	0.31555	0.63110	0.25000
C53	0.35100	0.64900	0.25000
H54	0.06400	0.34500	0.94800
H55	0.09700	0.40800	0.86100
H56	0.15100	0.43600	0.95500
H57	0.11700	0.40400	0.08700
H58	0.12700	0.39200	0.14600
H59	0.14000	0.31600	0.10600
H60	0.13000	0.32800	0.04800
H61	0.99000	0.26100	0.87000
H62	0.94200	0.22000	0.84000
H63	0.93900	0.29400	0.78100
H64	0.98700	0.33500	0.81200
H65	0.11200	0.20400	0.30500
H66	0.08200	0.14600	0.30100
H67	0.06000	0.03000	0.25000
H68	0.18700	0.46200	0.26200
H69	0.21700	0.52100	0.26200
H70	0.36300	0.63700	0.25000
C71	0.19891	0.51512	0.85806
C72	0.19539	0.52175	0.82204
C73	0.21964	0.55178	0.80605
C74	0.24739	0.57526	0.82592

C75	0.25103	0.56874	0.86200
C76	0.22680	0.53868	0.87811
H77	0.17413	0.50374	0.80658
H78	0.21689	0.55687	0.77817
H79	0.27247	0.58691	0.87726
H80	0.22988	0.53383	0.90612
Li81	0.06906	0.42501	0.94412
Li82	0.00492	0.27342	0.77589
Li83	0.26078	0.51863	0.81928
Li84	0.06203	0.31729	0.10326
Li85	0.33333	0.66667	0.32188
Zn86	0.69698	0.85328	0.21060
Zn87	0.63563	0.78432	0.24100
O88	0.66470	0.83235	0.25000
O89	0.63750	0.77900	0.19640
O90	0.67840	0.82670	0.17410
O91	0.80410	0.69410	0.79950
O92	0.76480	0.65330	0.76650
O93	0.73440	0.86200	0.22110
O94	0.59790	0.77550	0.25640
C95	0.61100	0.71930	0.95730
C96	0.63440	0.71470	0.93720
C97	0.62750	0.70340	0.90130
C98	0.59690	0.69680	0.88550
C99	0.57330	0.70130	0.90530
C100	0.58050	0.71260	0.94120
C101	0.61850	0.73150	0.99420
C102	0.62470	0.74200	0.02490
C103	0.63250	0.75530	0.06140
C104	0.61360	0.73570	0.09080
C105	0.62090	0.74880	0.12600
C106	0.64720	0.78200	0.13240
C107	0.66620	0.80150	0.10270
C108	0.65880	0.78820	0.06760
C109	0.65470	0.79660	0.16970
C110	0.65200	0.69890	0.88070
C111	0.67280	0.69540	0.86380
C112	0.69800	0.69130	0.84410
C113	0.73230	0.71200	0.85210
C114	0.75670	0.70750	0.83400
C115	0.74740	0.68230	0.80750
C116	0.71290	0.66200	0.79930
C117	0.68850	0.66650	0.81740
C118	0.77350	0.67640	0.78980
C119	0.54190	0.69500	0.88870

C120	0.51580	0.68990	0.87470
C121	0.75030	0.87515	0.25000
C122	0.78800	0.89400	0.25000
C123	0.80660	0.90900	0.28240
C124	0.84150	0.92590	0.27940
C125	0.86070	0.93035	0.25000
C126	0.89720	0.94860	0.25000
C127	0.92780	0.96390	0.25000
C128	0.96450	0.98225	0.25000
C129	0.98235	0.01765	0.25000
C130	0.58200	0.79100	0.25000
C131	0.54420	0.77210	0.25000
C132	0.52600	0.73720	0.25690
C133	0.49060	0.71950	0.25690
C134	0.47270	0.73635	0.25000
C135	0.43610	0.71805	0.25000
C136	0.40550	0.70275	0.25000
C137	0.36890	0.68445	0.25000
C138	0.35100	0.70200	0.25000
H139	0.65500	0.71900	0.94800
H140	0.59200	0.68900	0.86100
H141	0.56400	0.71500	0.95500
H142	0.59600	0.71300	0.08700
H143	0.60800	0.73500	0.14600
H144	0.68400	0.82400	0.10600
H145	0.67200	0.80200	0.04800
H146	0.73900	0.72900	0.87000
H147	0.78000	0.72200	0.84000
H148	0.70600	0.64500	0.78100
H149	0.66500	0.65200	0.81200
H150	0.79600	0.90800	0.30500
H151	0.85400	0.93600	0.30100
H152	0.97000	0.03000	0.25000
H153	0.53800	0.72500	0.26200
H154	0.47900	0.69600	0.26200
H155	0.36300	0.72600	0.25000
C156	0.48488	0.68379	0.85806
C157	0.47825	0.67365	0.82204
C158	0.44822	0.66786	0.80605
C159	0.42474	0.67213	0.82592
C160	0.43126	0.68229	0.86200
C161	0.46132	0.68812	0.87811
H162	0.49626	0.67038	0.80658
H163	0.44313	0.66002	0.77817
H164	0.41309	0.68556	0.87726

H165	0.46617	0.69604	0.90612
Li66	0.57499	0.64405	0.94412
Li67	0.72658	0.73151	0.77589
Li68	0.48137	0.74215	0.81928
Li69	0.68271	0.74474	0.10326
Zn70	0.14672	0.84370	0.21060
Zn71	0.21568	0.85131	0.24100
O172	0.16765	0.83235	0.25000
O173	0.22100	0.85850	0.19640
O174	0.17330	0.85170	0.17410
O175	0.30590	0.11000	0.79950
O176	0.34670	0.11150	0.76650
O177	0.13800	0.87240	0.22110
O178	0.22450	0.82240	0.25640
C179	0.28070	0.89170	0.95730
C180	0.28530	0.91970	0.93720
C181	0.29660	0.92410	0.90130
C182	0.30320	0.90010	0.88550
C183	0.29870	0.87200	0.90530
C184	0.28740	0.86790	0.94120
C185	0.26850	0.88700	0.99420
C186	0.25800	0.88270	0.02490
C187	0.24470	0.87720	0.06140
C188	0.26430	0.87790	0.09080
C189	0.25120	0.87210	0.12600
C190	0.21800	0.86520	0.13240
C191	0.19850	0.86470	0.10270
C192	0.21180	0.87060	0.06760
C193	0.20340	0.85810	0.16970
C194	0.30110	0.95310	0.88070
C195	0.30460	0.97740	0.86380
C196	0.30870	0.00670	0.84410
C197	0.28800	0.02030	0.85210
C198	0.29250	0.04920	0.83400
C199	0.31770	0.06510	0.80750
C200	0.33800	0.05090	0.79930
C201	0.33350	0.02200	0.81740
C202	0.32360	0.09710	0.78980
C203	0.30500	0.84690	0.88870
C204	0.31010	0.82590	0.87470
C205	0.12485	0.87515	0.25000
C206	0.10600	0.89400	0.25000
C207	0.09100	0.89760	0.28240
C208	0.07410	0.91560	0.27940
C209	0.06965	0.93035	0.25000

C210	0.05140	0.94860	0.25000
C211	0.03610	0.96390	0.25000
C212	0.01775	0.98225	0.25000
C213	0.98235	0.96470	0.25000
C214	0.20900	0.79100	0.25000
C215	0.22790	0.77210	0.25000
C216	0.26280	0.78880	0.25690
C217	0.28050	0.77110	0.25690
C218	0.26365	0.73635	0.25000
C219	0.28195	0.71805	0.25000
C220	0.29725	0.70275	0.25000
C221	0.31555	0.68445	0.25000
C222	0.29800	0.64900	0.25000
H223	0.28100	0.93600	0.94800
H224	0.31100	0.90300	0.86100
H225	0.28500	0.84900	0.95500
H226	0.28700	0.88300	0.08700
H227	0.26500	0.87300	0.14600
H228	0.17600	0.86000	0.10600
H229	0.19800	0.87000	0.04800
H230	0.27100	0.01000	0.87000
H231	0.27800	0.05800	0.84000
H232	0.35500	0.06100	0.78100
H233	0.34800	0.01300	0.81200
H234	0.09200	0.88800	0.30500
H235	0.06400	0.91800	0.30100
H236	0.97000	0.94000	0.25000
H237	0.27500	0.81300	0.26200
H238	0.30400	0.78300	0.26200
H239	0.27400	0.63700	0.25000
C240	0.31621	0.80109	0.85806
C241	0.32635	0.80461	0.82204
C242	0.33214	0.78036	0.80605
C243	0.32787	0.75261	0.82592
C244	0.31771	0.74897	0.86200
C245	0.31188	0.77320	0.87811
H246	0.32962	0.82587	0.80658
H247	0.33998	0.78311	0.77817
H248	0.31444	0.72753	0.87726
H249	0.30396	0.77012	0.90612
Li50	0.35595	0.93094	0.94412
Li51	0.26849	0.99508	0.77589
Li52	0.25785	0.73922	0.81928
Li53	0.25526	0.93797	0.10326
Zn54	0.69698	0.84370	0.28940

Zn55	0.63563	0.85131	0.25900
O256	0.63750	0.85850	0.30360
O257	0.67840	0.85170	0.32590
O258	0.80410	0.11000	0.70050
O259	0.76480	0.11150	0.73350
O260	0.73440	0.87240	0.27890
O261	0.59790	0.82240	0.24360
C262	0.61100	0.89170	0.54270
C263	0.63440	0.91970	0.56280
C264	0.62750	0.92410	0.59870
C265	0.59690	0.90010	0.61450
C266	0.57330	0.87200	0.59470
C267	0.58050	0.86790	0.55880
C268	0.61850	0.88700	0.50580
C269	0.62470	0.88270	0.47510
C270	0.63250	0.87720	0.43860
C271	0.61360	0.87790	0.40920
C272	0.62090	0.87210	0.37400
C273	0.64720	0.86520	0.36760
C274	0.66620	0.86470	0.39730
C275	0.65880	0.87060	0.43240
C276	0.65470	0.85810	0.33030
C277	0.65200	0.95310	0.61930
C278	0.67280	0.97740	0.63620
C279	0.69800	0.00670	0.65590
C280	0.73230	0.02030	0.64790
C281	0.75670	0.04920	0.66600
C282	0.74740	0.06510	0.69250
C283	0.71290	0.05090	0.70070
C284	0.68850	0.02200	0.68260
C285	0.77350	0.09710	0.71020
C286	0.54190	0.84690	0.61130
C287	0.51580	0.82590	0.62530
C288	0.80660	0.89760	0.21760
C289	0.84150	0.91560	0.22060
C290	0.52600	0.78880	0.24310
C291	0.49060	0.77110	0.24310
H292	0.65500	0.93600	0.55200
H293	0.59200	0.90300	0.63900
H294	0.56400	0.84900	0.54500
H295	0.59600	0.88300	0.41300
H296	0.60800	0.87300	0.35400
H297	0.68400	0.86000	0.39400
H298	0.67200	0.87000	0.45200
H299	0.73900	0.01000	0.63000

H300	0.78000	0.05800	0.66000
H301	0.70600	0.06100	0.71900
H302	0.66500	0.01300	0.68800
H303	0.79600	0.88800	0.19500
H304	0.85400	0.91800	0.19900
H305	0.53800	0.81300	0.23800
H306	0.47900	0.78300	0.23800
C307	0.48488	0.80109	0.64194
C308	0.47825	0.80461	0.67796
C309	0.44822	0.78036	0.69395
C310	0.42474	0.75261	0.67408
C311	0.43126	0.74897	0.63800
C312	0.46132	0.77320	0.62189
H313	0.49626	0.82587	0.69342
H314	0.44313	0.78311	0.72183
H315	0.41309	0.72753	0.62274
H316	0.46617	0.77012	0.59388
Li17	0.57499	0.93094	0.55588
Li18	0.72658	0.99508	0.72411
Li19	0.48137	0.73922	0.68072
Li20	0.68271	0.93797	0.39674
Li21	0.51062	0.74288	0.17888
Li22	0.82213	0.96869	0.23497
Li23	0.00000	0.00000	0.32188
Zn24	0.14672	0.30302	0.28940
Zn25	0.21568	0.36437	0.25900
O326	0.22100	0.36250	0.30360
O327	0.17330	0.32160	0.32590
O328	0.30590	0.19590	0.70050
O329	0.34670	0.23520	0.73350
O330	0.13800	0.26560	0.27890
O331	0.22450	0.40210	0.24360
C332	0.28070	0.38900	0.54270
C333	0.28530	0.36560	0.56280
C334	0.29660	0.37250	0.59870
C335	0.30320	0.40310	0.61450
C336	0.29870	0.42670	0.59470
C337	0.28740	0.41950	0.55880
C338	0.26850	0.38150	0.50580
C339	0.25800	0.37530	0.47510
C340	0.24470	0.36750	0.43860
C341	0.26430	0.38640	0.40920
C342	0.25120	0.37910	0.37400
C343	0.21800	0.35280	0.36760
C344	0.19850	0.33380	0.39730

C345	0.21180	0.34120	0.43240
C346	0.20340	0.34530	0.33030
C347	0.30110	0.34800	0.61930
C348	0.30460	0.32720	0.63620
C349	0.30870	0.30200	0.65590
C350	0.28800	0.26770	0.64790
C351	0.29250	0.24330	0.66600
C352	0.31770	0.25260	0.69250
C353	0.33800	0.28710	0.70070
C354	0.33350	0.31150	0.68260
C355	0.32360	0.22650	0.71020
C356	0.30500	0.45810	0.61130
C357	0.31010	0.48420	0.62530
C358	0.09100	0.19340	0.21760
C359	0.07410	0.15850	0.22060
C360	0.26280	0.47400	0.24310
C361	0.28050	0.50940	0.24310
H362	0.28100	0.34500	0.55200
H363	0.31100	0.40800	0.63900
H364	0.28500	0.43600	0.54500
H365	0.28700	0.40400	0.41300
H366	0.26500	0.39200	0.35400
H367	0.17600	0.31600	0.39400
H368	0.19800	0.32800	0.45200
H369	0.27100	0.26100	0.63000
H370	0.27800	0.22000	0.66000
H371	0.35500	0.29400	0.71900
H372	0.34800	0.33500	0.68800
H373	0.09200	0.20400	0.19500
H374	0.06400	0.14600	0.19900
H375	0.27500	0.46200	0.23800
H376	0.30400	0.52100	0.23800
C377	0.31621	0.51512	0.64194
C378	0.32635	0.52175	0.67796
C379	0.33214	0.55178	0.69395
C380	0.32787	0.57526	0.67408
C381	0.31771	0.56874	0.63800
C382	0.31188	0.53868	0.62189
H383	0.32962	0.50374	0.69342
H384	0.33998	0.55687	0.72183
H385	0.31444	0.58691	0.62274
H386	0.30396	0.53383	0.59388
Li87	0.35595	0.42501	0.55588
Li88	0.26849	0.27342	0.72411
Li89	0.25785	0.51863	0.68072

Li90	0.25526	0.31729	0.39674
Li91	0.23226	0.48938	0.17888
Li92	0.14656	0.17787	0.23497
Zn93	0.15630	0.85328	0.28940
Zn94	0.14869	0.78432	0.25900
O395	0.14150	0.77900	0.30360
O396	0.14830	0.82670	0.32590
O397	0.89000	0.69410	0.70050
O398	0.88850	0.65330	0.73350
O399	0.12760	0.86200	0.27890
O400	0.17760	0.77550	0.24360
C401	0.10830	0.71930	0.54270
C402	0.08030	0.71470	0.56280
C403	0.07590	0.70340	0.59870
C404	0.09990	0.69680	0.61450
C405	0.12800	0.70130	0.59470
C406	0.13210	0.71260	0.55880
C407	0.11300	0.73150	0.50580
C408	0.11730	0.74200	0.47510
C409	0.12280	0.75530	0.43860
C410	0.12210	0.73570	0.40920
C411	0.12790	0.74880	0.37400
C412	0.13480	0.78200	0.36760
C413	0.13530	0.80150	0.39730
C414	0.12940	0.78820	0.43240
C415	0.14190	0.79660	0.33030
C416	0.04690	0.69890	0.61930
C417	0.02260	0.69540	0.63620
C418	0.99330	0.69130	0.65590
C419	0.97970	0.71200	0.64790
C420	0.95080	0.70750	0.66600
C421	0.93490	0.68230	0.69250
C422	0.94910	0.66200	0.70070
C423	0.97800	0.66650	0.68260
C424	0.90290	0.67640	0.71020
C425	0.15310	0.69500	0.61130
C426	0.17410	0.68990	0.62530
C427	0.10240	0.90900	0.21760
C428	0.08440	0.92590	0.22060
C429	0.21120	0.73720	0.24310
C430	0.22890	0.71950	0.24310
H431	0.06400	0.71900	0.55200
H432	0.09700	0.68900	0.63900
H433	0.15100	0.71500	0.54500
H434	0.11700	0.71300	0.41300

H435	0.12700	0.73500	0.35400
H436	0.14000	0.82400	0.39400
H437	0.13000	0.80200	0.45200
H438	0.99000	0.72900	0.63000
H439	0.94200	0.72200	0.66000
H440	0.93900	0.64500	0.71900
H441	0.98700	0.65200	0.68800
H442	0.11200	0.90800	0.19500
H443	0.08200	0.93600	0.19900
H444	0.18700	0.72500	0.23800
H445	0.21700	0.69600	0.23800
C446	0.19891	0.68379	0.64194
C447	0.19539	0.67365	0.67796
C448	0.21964	0.66786	0.69395
C449	0.24739	0.67213	0.67408
C450	0.25103	0.68229	0.63800
C451	0.22680	0.68812	0.62189
H452	0.17413	0.67038	0.69342
H453	0.21689	0.66002	0.72183
H454	0.27247	0.68556	0.62274
H455	0.22988	0.69604	0.59388
Li56	0.06906	0.64405	0.55588
Li57	0.00492	0.73151	0.72411
Li58	0.26078	0.74215	0.68072
Li59	0.06203	0.74474	0.39674
Li60	0.25712	0.76774	0.17888
Li61	0.03131	0.85344	0.23497
Zn62	0.84370	0.69698	0.78940
Zn63	0.85131	0.63563	0.75900
O464	0.83235	0.66470	0.75000
O465	0.85850	0.63750	0.80360
O466	0.85170	0.67840	0.82590
O467	0.11000	0.80410	0.20050
O468	0.11150	0.76480	0.23350
O469	0.87240	0.73440	0.77890
O470	0.82240	0.59790	0.74360
C471	0.89170	0.61100	0.04270
C472	0.91970	0.63440	0.06280
C473	0.92410	0.62750	0.09870
C474	0.90010	0.59690	0.11450
C475	0.87200	0.57330	0.09470
C476	0.86790	0.58050	0.05880
C477	0.88700	0.61850	0.00580
C478	0.88270	0.62470	0.97510
C479	0.87720	0.63250	0.93860

C480	0.87790	0.61360	0.90920
C481	0.87210	0.62090	0.87400
C482	0.86520	0.64720	0.86760
C483	0.86470	0.66620	0.89730
C484	0.87060	0.65880	0.93240
C485	0.85810	0.65470	0.83030
C486	0.95310	0.65200	0.11930
C487	0.97740	0.67280	0.13620
C488	0.00670	0.69800	0.15590
C489	0.02030	0.73230	0.14790
C490	0.04920	0.75670	0.16600
C491	0.06510	0.74740	0.19250
C492	0.05090	0.71290	0.20070
C493	0.02200	0.68850	0.18260
C494	0.09710	0.77350	0.21020
C495	0.84690	0.54190	0.11130
C496	0.82590	0.51580	0.12530
C497	0.87515	0.75030	0.75000
C498	0.89400	0.78800	0.75000
C499	0.89760	0.80660	0.71760
C500	0.91560	0.84150	0.72060
C501	0.93035	0.86070	0.75000
C502	0.94860	0.89720	0.75000
C503	0.96390	0.92780	0.75000
C504	0.98225	0.96450	0.75000
C505	0.96470	0.98235	0.75000
C506	0.79100	0.58200	0.75000
C507	0.77210	0.54420	0.75000
C508	0.78880	0.52600	0.74310
C509	0.77110	0.49060	0.74310
C510	0.73635	0.47270	0.75000
C511	0.71805	0.43610	0.75000
C512	0.70275	0.40550	0.75000
C513	0.68445	0.36890	0.75000
C514	0.64900	0.35100	0.75000
H515	0.93600	0.65500	0.05200
H516	0.90300	0.59200	0.13900
H517	0.84900	0.56400	0.04500
H518	0.88300	0.59600	0.91300
H519	0.87300	0.60800	0.85400
H520	0.86000	0.68400	0.89400
H521	0.87000	0.67200	0.95200
H522	0.01000	0.73900	0.13000
H523	0.05800	0.78000	0.16000
H524	0.06100	0.70600	0.21900

H525	0.01300	0.66500	0.18800
H526	0.88800	0.79600	0.69500
H527	0.91800	0.85400	0.69900
H528	0.94000	0.97000	0.75000
H529	0.81300	0.53800	0.73800
H530	0.78300	0.47900	0.73800
H531	0.63700	0.36300	0.75000
C532	0.80109	0.48488	0.14194
C533	0.80461	0.47825	0.17796
C534	0.78036	0.44822	0.19395
C535	0.75261	0.42474	0.17408
C536	0.74897	0.43126	0.13800
C537	0.77320	0.46132	0.12189
H538	0.82587	0.49626	0.19342
H539	0.78311	0.44313	0.22183
H540	0.72753	0.41309	0.12274
H541	0.77012	0.46617	0.09388
Li42	0.93094	0.57499	0.05588
Li43	0.99508	0.72658	0.22411
Li44	0.73922	0.48137	0.18072
Li45	0.93797	0.68271	0.89674
Li46	0.74288	0.51062	0.67888
Li47	0.96869	0.82213	0.73497
Li48	0.00000	0.00000	0.82188
Zn49	0.30302	0.14672	0.78940
Zn50	0.36437	0.21568	0.75900
O551	0.33530	0.16765	0.75000
O552	0.36250	0.22100	0.80360
O553	0.32160	0.17330	0.82590
O554	0.19590	0.30590	0.20050
O555	0.23520	0.34670	0.23350
O556	0.26560	0.13800	0.77890
O557	0.40210	0.22450	0.74360
C558	0.38900	0.28070	0.04270
C559	0.36560	0.28530	0.06280
C560	0.37250	0.29660	0.09870
C561	0.40310	0.30320	0.11450
C562	0.42670	0.29870	0.09470
C563	0.41950	0.28740	0.05880
C564	0.38150	0.26850	0.00580
C565	0.37530	0.25800	0.97510
C566	0.36750	0.24470	0.93860
C567	0.38640	0.26430	0.90920
C568	0.37910	0.25120	0.87400
C569	0.35280	0.21800	0.86760

C570	0.33380	0.19850	0.89730
C571	0.34120	0.21180	0.93240
C572	0.34530	0.20340	0.83030
C573	0.34800	0.30110	0.11930
C574	0.32720	0.30460	0.13620
C575	0.30200	0.30870	0.15590
C576	0.26770	0.28800	0.14790
C577	0.24330	0.29250	0.16600
C578	0.25260	0.31770	0.19250
C579	0.28710	0.33800	0.20070
C580	0.31150	0.33350	0.18260
C581	0.22650	0.32360	0.21020
C582	0.45810	0.30500	0.11130
C583	0.48420	0.31010	0.12530
C584	0.24970	0.12485	0.75000
C585	0.21200	0.10600	0.75000
C586	0.19340	0.09100	0.71760
C587	0.15850	0.07410	0.72060
C588	0.13930	0.06965	0.75000
C589	0.10280	0.05140	0.75000
C590	0.07220	0.03610	0.75000
C591	0.03550	0.01775	0.75000
C592	0.01765	0.98235	0.75000
C593	0.41800	0.20900	0.75000
C594	0.45580	0.22790	0.75000
C595	0.47400	0.26280	0.74310
C596	0.50940	0.28050	0.74310
C597	0.52730	0.26365	0.75000
C598	0.56390	0.28195	0.75000
C599	0.59450	0.29725	0.75000
C600	0.63110	0.31555	0.75000
C601	0.64900	0.29800	0.75000
H602	0.34500	0.28100	0.05200
H603	0.40800	0.31100	0.13900
H604	0.43600	0.28500	0.04500
H605	0.40400	0.28700	0.91300
H606	0.39200	0.26500	0.85400
H607	0.31600	0.17600	0.89400
H608	0.32800	0.19800	0.95200
H609	0.26100	0.27100	0.13000
H610	0.22000	0.27800	0.16000
H611	0.29400	0.35500	0.21900
H612	0.33500	0.34800	0.18800
H613	0.20400	0.09200	0.69500
H614	0.14600	0.06400	0.69900

H615	0.03000	0.97000	0.75000
H616	0.46200	0.27500	0.73800
H617	0.52100	0.30400	0.73800
H618	0.63700	0.27400	0.75000
C619	0.51512	0.31621	0.14194
C620	0.52175	0.32635	0.17796
C621	0.55178	0.33214	0.19395
C622	0.57526	0.32787	0.17408
C623	0.56874	0.31771	0.13800
C624	0.53868	0.31188	0.12189
H625	0.50374	0.32962	0.19342
H626	0.55687	0.33998	0.22183
H627	0.58691	0.31444	0.12274
H628	0.53383	0.30396	0.09388
Li29	0.42501	0.35595	0.05588
Li30	0.27342	0.26849	0.22411
Li31	0.51863	0.25785	0.18072
Li32	0.31729	0.25526	0.89674
Li33	0.48938	0.23226	0.67888
Li34	0.17787	0.14656	0.73497
Zn35	0.85328	0.15630	0.78940
Zn36	0.78432	0.14869	0.75900
O637	0.83235	0.16765	0.75000
O638	0.77900	0.14150	0.80360
O639	0.82670	0.14830	0.82590
O640	0.69410	0.89000	0.20050
O641	0.65330	0.88850	0.23350
O642	0.86200	0.12760	0.77890
O643	0.77550	0.17760	0.74360
C644	0.71930	0.10830	0.04270
C645	0.71470	0.08030	0.06280
C646	0.70340	0.07590	0.09870
C647	0.69680	0.09990	0.11450
C648	0.70130	0.12800	0.09470
C649	0.71260	0.13210	0.05880
C650	0.73150	0.11300	0.00580
C651	0.74200	0.11730	0.97510
C652	0.75530	0.12280	0.93860
C653	0.73570	0.12210	0.90920
C654	0.74880	0.12790	0.87400
C655	0.78200	0.13480	0.86760
C656	0.80150	0.13530	0.89730
C657	0.78820	0.12940	0.93240
C658	0.79660	0.14190	0.83030
C659	0.69890	0.04690	0.11930

C660	0.69540	0.02260	0.13620
C661	0.69130	0.99330	0.15590
C662	0.71200	0.97970	0.14790
C663	0.70750	0.95080	0.16600
C664	0.68230	0.93490	0.19250
C665	0.66200	0.94910	0.20070
C666	0.66650	0.97800	0.18260
C667	0.67640	0.90290	0.21020
C668	0.69500	0.15310	0.11130
C669	0.68990	0.17410	0.12530
C670	0.87515	0.12485	0.75000
C671	0.89400	0.10600	0.75000
C672	0.90900	0.10240	0.71760
C673	0.92590	0.08440	0.72060
C674	0.93035	0.06965	0.75000
C675	0.94860	0.05140	0.75000
C676	0.96390	0.03610	0.75000
C677	0.98225	0.01775	0.75000
C678	0.01765	0.03530	0.75000
C679	0.79100	0.20900	0.75000
C680	0.77210	0.22790	0.75000
C681	0.73720	0.21120	0.74310
C682	0.71950	0.22890	0.74310
C683	0.73635	0.26365	0.75000
C684	0.71805	0.28195	0.75000
C685	0.70275	0.29725	0.75000
C686	0.68445	0.31555	0.75000
C687	0.70200	0.35100	0.75000
H688	0.71900	0.06400	0.05200
H689	0.68900	0.09700	0.13900
H690	0.71500	0.15100	0.04500
H691	0.71300	0.11700	0.91300
H692	0.73500	0.12700	0.85400
H693	0.82400	0.14000	0.89400
H694	0.80200	0.13000	0.95200
H695	0.72900	0.99000	0.13000
H696	0.72200	0.94200	0.16000
H697	0.64500	0.93900	0.21900
H698	0.65200	0.98700	0.18800
H699	0.90800	0.11200	0.69500
H700	0.93600	0.08200	0.69900
H701	0.03000	0.06000	0.75000
H702	0.72500	0.18700	0.73800
H703	0.69600	0.21700	0.73800
H704	0.72600	0.36300	0.75000

C705	0.68379	0.19891	0.14194
C706	0.67365	0.19539	0.17796
C707	0.66786	0.21964	0.19395
C708	0.67213	0.24739	0.17408
C709	0.68229	0.25103	0.13800
C710	0.68812	0.22680	0.12189
H711	0.67038	0.17413	0.19342
H712	0.66002	0.21689	0.22183
H713	0.68556	0.27247	0.12274
H714	0.69604	0.22988	0.09388
Li15	0.64405	0.06906	0.05588
Li16	0.73151	0.00492	0.22411
Li17	0.74215	0.26078	0.18072
Li18	0.74474	0.06203	0.89674
Li19	0.76774	0.25712	0.67888
Li20	0.85344	0.03131	0.73497
Zn21	0.30302	0.15630	0.71060
Zn22	0.36437	0.14869	0.74100
O723	0.36250	0.14150	0.69640
O724	0.32160	0.14830	0.67410
O725	0.19590	0.89000	0.29950
O726	0.23520	0.88850	0.26650
O727	0.26560	0.12760	0.72110
O728	0.40210	0.17760	0.75640
C729	0.38900	0.10830	0.45730
C730	0.36560	0.08030	0.43720
C731	0.37250	0.07590	0.40130
C732	0.40310	0.09990	0.38550
C733	0.42670	0.12800	0.40530
C734	0.41950	0.13210	0.44120
C735	0.38150	0.11300	0.49420
C736	0.37530	0.11730	0.52490
C737	0.36750	0.12280	0.56140
C738	0.38640	0.12210	0.59080
C739	0.37910	0.12790	0.62600
C740	0.35280	0.13480	0.63240
C741	0.33380	0.13530	0.60270
C742	0.34120	0.12940	0.56760
C743	0.34530	0.14190	0.66970
C744	0.34800	0.04690	0.38070
C745	0.32720	0.02260	0.36380
C746	0.30200	0.99330	0.34410
C747	0.26770	0.97970	0.35210
C748	0.24330	0.95080	0.33400
C749	0.25260	0.93490	0.30750

C750	0.28710	0.94910	0.29930
C751	0.31150	0.97800	0.31740
C752	0.22650	0.90290	0.28980
C753	0.45810	0.15310	0.38870
C754	0.48420	0.17410	0.37470
C755	0.19340	0.10240	0.78240
C756	0.15850	0.08440	0.77940
C757	0.47400	0.21120	0.75690
C758	0.50940	0.22890	0.75690
H759	0.34500	0.06400	0.44800
H760	0.40800	0.09700	0.36100
H761	0.43600	0.15100	0.45500
H762	0.40400	0.11700	0.58700
H763	0.39200	0.12700	0.64600
H764	0.31600	0.14000	0.60600
H765	0.32800	0.13000	0.54800
H766	0.26100	0.99000	0.37000
H767	0.22000	0.94200	0.34000
H768	0.29400	0.93900	0.28100
H769	0.33500	0.98700	0.31200
H770	0.20400	0.11200	0.80500
H771	0.14600	0.08200	0.80100
H772	0.46200	0.18700	0.76200
H773	0.52100	0.21700	0.76200
C774	0.51512	0.19891	0.35806
C775	0.52175	0.19539	0.32204
C776	0.55178	0.21964	0.30605
C777	0.57526	0.24739	0.32592
C778	0.56874	0.25103	0.36200
C779	0.53868	0.22680	0.37811
H780	0.50374	0.17413	0.30658
H781	0.55687	0.21689	0.27817
H782	0.58691	0.27247	0.37726
H783	0.53383	0.22988	0.40612
Li84	0.42501	0.06906	0.44412
Li85	0.27342	0.00492	0.27589
Li86	0.51863	0.26078	0.31928
Li87	0.31729	0.06203	0.60326
Li88	0.66667	0.33333	0.82188
Zn89	0.85328	0.69698	0.71060
Zn90	0.78432	0.63563	0.74100
O791	0.77900	0.63750	0.69640
O792	0.82670	0.67840	0.67410
O793	0.69410	0.80410	0.29950
O794	0.65330	0.76480	0.26650

O795	0.86200	0.73440	0.72110
O796	0.77550	0.59790	0.75640
C797	0.71930	0.61100	0.45730
C798	0.71470	0.63440	0.43720
C799	0.70340	0.62750	0.40130
C800	0.69680	0.59690	0.38550
C801	0.70130	0.57330	0.40530
C802	0.71260	0.58050	0.44120
C803	0.73150	0.61850	0.49420
C804	0.74200	0.62470	0.52490
C805	0.75530	0.63250	0.56140
C806	0.73570	0.61360	0.59080
C807	0.74880	0.62090	0.62600
C808	0.78200	0.64720	0.63240
C809	0.80150	0.66620	0.60270
C810	0.78820	0.65880	0.56760
C811	0.79660	0.65470	0.66970
C812	0.69890	0.65200	0.38070
C813	0.69540	0.67280	0.36380
C814	0.69130	0.69800	0.34410
C815	0.71200	0.73230	0.35210
C816	0.70750	0.75670	0.33400
C817	0.68230	0.74740	0.30750
C818	0.66200	0.71290	0.29930
C819	0.66650	0.68850	0.31740
C820	0.67640	0.77350	0.28980
C821	0.69500	0.54190	0.38870
C822	0.68990	0.51580	0.37470
C823	0.90900	0.80660	0.78240
C824	0.92590	0.84150	0.77940
C825	0.73720	0.52600	0.75690
C826	0.71950	0.49060	0.75690
H827	0.71900	0.65500	0.44800
H828	0.68900	0.59200	0.36100
H829	0.71500	0.56400	0.45500
H830	0.71300	0.59600	0.58700
H831	0.73500	0.60800	0.64600
H832	0.82400	0.68400	0.60600
H833	0.80200	0.67200	0.54800
H834	0.72900	0.73900	0.37000
H835	0.72200	0.78000	0.34000
H836	0.64500	0.70600	0.28100
H837	0.65200	0.66500	0.31200
H838	0.90800	0.79600	0.80500
H839	0.93600	0.85400	0.80100

H840	0.72500	0.53800	0.76200
H841	0.69600	0.47900	0.76200
C842	0.68379	0.48488	0.35806
C843	0.67365	0.47825	0.32204
C844	0.66786	0.44822	0.30605
C845	0.67213	0.42474	0.32592
C846	0.68229	0.43126	0.36200
C847	0.68812	0.46132	0.37811
H848	0.67038	0.49626	0.30658
H849	0.66002	0.44313	0.27817
H850	0.68556	0.41309	0.37726
H851	0.69604	0.46617	0.40612
Li52	0.64405	0.57499	0.44412
Li53	0.73151	0.72658	0.27589
Li54	0.74215	0.48137	0.31928
Li55	0.74474	0.68271	0.60326
Zn56	0.84370	0.14672	0.71060
Zn57	0.85131	0.21568	0.74100
O858	0.85850	0.22100	0.69640
O859	0.85170	0.17330	0.67410
O860	0.11000	0.30590	0.29950
O861	0.11150	0.34670	0.26650
O862	0.87240	0.13800	0.72110
O863	0.82240	0.22450	0.75640
C864	0.89170	0.28070	0.45730
C865	0.91970	0.28530	0.43720
C866	0.92410	0.29660	0.40130
C867	0.90010	0.30320	0.38550
C868	0.87200	0.29870	0.40530
C869	0.86790	0.28740	0.44120
C870	0.88700	0.26850	0.49420
C871	0.88270	0.25800	0.52490
C872	0.87720	0.24470	0.56140
C873	0.87790	0.26430	0.59080
C874	0.87210	0.25120	0.62600
C875	0.86520	0.21800	0.63240
C876	0.86470	0.19850	0.60270
C877	0.87060	0.21180	0.56760
C878	0.85810	0.20340	0.66970
C879	0.95310	0.30110	0.38070
C880	0.97740	0.30460	0.36380
C881	0.00670	0.30870	0.34410
C882	0.02030	0.28800	0.35210
C883	0.04920	0.29250	0.33400
C884	0.06510	0.31770	0.30750

C885	0.05090	0.33800	0.29930
C886	0.02200	0.33350	0.31740
C887	0.09710	0.32360	0.28980
C888	0.84690	0.30500	0.38870
C889	0.82590	0.31010	0.37470
C890	0.89760	0.09100	0.78240
C891	0.91560	0.07410	0.77940
C892	0.78880	0.26280	0.75690
C893	0.77110	0.28050	0.75690
H894	0.93600	0.28100	0.44800
H895	0.90300	0.31100	0.36100
H896	0.84900	0.28500	0.45500
H897	0.88300	0.28700	0.58700
H898	0.87300	0.26500	0.64600
H899	0.86000	0.17600	0.60600
H900	0.87000	0.19800	0.54800
H901	0.01000	0.27100	0.37000
H902	0.05800	0.27800	0.34000
H903	0.06100	0.35500	0.28100
H904	0.01300	0.34800	0.31200
H905	0.88800	0.09200	0.80500
H906	0.91800	0.06400	0.80100
H907	0.81300	0.27500	0.76200
H908	0.78300	0.30400	0.76200
C909	0.80109	0.31621	0.35806
C910	0.80461	0.32635	0.32204
C911	0.78036	0.33214	0.30605
C912	0.75261	0.32787	0.32592
C913	0.74897	0.31771	0.36200
C914	0.77320	0.31188	0.37811
H915	0.82587	0.32962	0.30658
H916	0.78311	0.33998	0.27817
H917	0.72753	0.31444	0.37726
H918	0.77012	0.30396	0.40612
Li19	0.93094	0.35595	0.44412
Li20	0.99508	0.26849	0.27589
Li21	0.73922	0.25785	0.31928
Li22	0.93797	0.25526	0.60326
C923	0.27237	0.60293	0.80565
C924	0.32945	0.72811	0.80236
C925	0.39726	0.67057	0.80437
C926	0.27279	0.66969	0.69845
C927	0.39663	0.72436	0.69771
C928	0.32764	0.60101	0.70027
Zn29	0.36940	0.70522	0.76784

Zn30	0.33491	0.62988	0.76939
Zn31	0.29403	0.66428	0.76847
Zn32	0.33232	0.66518	0.70187
O933	0.39657	0.72964	0.73135
O934	0.37206	0.69867	0.68287
O935	0.33267	0.66615	0.75177
O936	0.32633	0.62504	0.68436
O937	0.33269	0.60193	0.73405
O938	0.26842	0.66541	0.73232
O939	0.39695	0.69748	0.79654
O940	0.37334	0.64195	0.79437
O941	0.35792	0.73256	0.79207
O942	0.30245	0.70060	0.79563
O943	0.26760	0.62655	0.79465
O944	0.29955	0.60305	0.79820
O945	0.29827	0.67070	0.68321
C946	0.66865	0.27311	0.19103
C947	0.59934	0.27017	0.29647
C948	0.60318	0.33129	0.19376
C949	0.66981	0.39488	0.30158
C950	0.72396	0.32412	0.29859
C951	0.72686	0.39638	0.19659
Zn52	0.70413	0.36679	0.26506
Zn53	0.66165	0.29178	0.26167
Zn54	0.62908	0.33437	0.26364
Zn55	0.66611	0.33350	0.19684
O956	0.73058	0.39476	0.23033
O957	0.70125	0.37321	0.18019
O958	0.66524	0.33161	0.24667
O959	0.67081	0.29951	0.17687
O960	0.66331	0.26739	0.22460
O961	0.60289	0.33465	0.22774
O962	0.72952	0.35327	0.28963
O963	0.69647	0.29786	0.29002
O964	0.69648	0.39395	0.29426
O965	0.64122	0.37193	0.29028
O966	0.60055	0.29809	0.29034
O967	0.62282	0.26508	0.28576
O968	0.62735	0.32994	0.17828

8.8 MOF205-Li

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Name
MOF205-Li

Space group symmetry
P 1

a = b = c =  30.353  A
 alpha = betha = gamma = 90.000
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Atom	x	y	z
Zn1	0.50000	0.94806	0.21258
O2	0.50000	0.00000	0.25000
O3	0.55094	0.91182	0.22472
C4	0.58289	0.91711	0.25000
C5	0.61769	0.88231	0.25000
C6	0.61051	0.84098	0.23293
H7	0.58310	0.83490	0.22060
C8	0.64162	0.80846	0.23315
H9	0.63500	0.78070	0.22200
C10	0.68284	0.81716	0.25000
C11	0.71702	0.78298	0.25000
C12	0.75000	0.78211	0.28211
H13	0.75000	0.80380	0.30380
O14	0.50000	0.96297	0.15039
C15	0.50000	0.00000	0.13094
Zn16	0.50000	0.05194	0.21258
O17	0.44906	0.08818	0.22472
C18	0.41711	0.08289	0.25000
C19	0.38231	0.11769	0.25000
C20	0.38949	0.15902	0.23293
H21	0.41690	0.16510	0.22060
C22	0.35838	0.19154	0.23315
H23	0.36500	0.21930	0.22200
C24	0.31716	0.18284	0.25000
C25	0.28298	0.21702	0.25000
C26	0.25000	0.21789	0.28211
H27	0.25000	0.19620	0.30380
O28	0.50000	0.03703	0.15039
Zn29	0.50000	0.94806	0.78742
O30	0.50000	0.00000	0.75000
O31	0.44906	0.91182	0.77528
C32	0.41711	0.91711	0.75000

C33	0.38231	0.88231	0.75000
C34	0.38949	0.84098	0.76707
H35	0.41690	0.83490	0.77940
C36	0.35838	0.80846	0.76685
H37	0.36500	0.78070	0.77800
C38	0.31716	0.81716	0.75000
C39	0.28298	0.78298	0.75000
C40	0.25000	0.78211	0.71789
H41	0.25000	0.80380	0.69620
O42	0.50000	0.96297	0.84961
C43	0.50000	0.00000	0.86906
Zn44	0.50000	0.05194	0.78742
O45	0.55094	0.08818	0.77528
C46	0.58289	0.08289	0.75000
C47	0.61769	0.11769	0.75000
C48	0.61051	0.15902	0.76707
H49	0.58310	0.16510	0.77940
C50	0.64162	0.19154	0.76685
H51	0.63500	0.21930	0.77800
C52	0.68284	0.18284	0.75000
C53	0.71702	0.21702	0.75000
C54	0.75000	0.21789	0.71789
H55	0.75000	0.19620	0.69620
O56	0.50000	0.03703	0.84961
Zn57	0.21258	0.50000	0.94806
O58	0.25000	0.50000	0.00000
O59	0.22472	0.55094	0.91182
C60	0.25000	0.58289	0.91711
C61	0.25000	0.61769	0.88231
C62	0.23293	0.61051	0.84098
H63	0.22060	0.58310	0.83490
C64	0.23315	0.64162	0.80846
H65	0.22200	0.63500	0.78070
C66	0.25000	0.68284	0.81716
C67	0.25000	0.71702	0.78298
C68	0.28211	0.75000	0.78211
H69	0.30380	0.75000	0.80380
O70	0.15039	0.50000	0.96297
C71	0.13094	0.50000	0.00000
Zn72	0.21258	0.50000	0.05194
O73	0.22472	0.44906	0.08818
C74	0.25000	0.41711	0.08289
C75	0.25000	0.38231	0.11769
C76	0.23293	0.38949	0.15902
H77	0.22060	0.41690	0.16510

C78	0.23315	0.35838	0.19154
H79	0.22200	0.36500	0.21930
C80	0.25000	0.31716	0.18284
C81	0.25000	0.28298	0.21702
C82	0.28211	0.25000	0.21789
H83	0.30380	0.25000	0.19620
O84	0.15039	0.50000	0.03703
Zn85	0.78742	0.50000	0.94806
O86	0.75000	0.50000	0.00000
O87	0.77528	0.44906	0.91182
C88	0.75000	0.41711	0.91711
C89	0.75000	0.38231	0.88231
C90	0.76707	0.38949	0.84098
H91	0.77940	0.41690	0.83490
C92	0.76685	0.35838	0.80846
H93	0.77800	0.36500	0.78070
C94	0.75000	0.31716	0.81716
C95	0.75000	0.28298	0.78298
C96	0.71789	0.25000	0.78211
H97	0.69620	0.25000	0.80380
O98	0.84961	0.50000	0.96297
C99	0.86906	0.50000	0.00000
Zn0	0.78742	0.50000	0.05194
O101	0.77528	0.55094	0.08818
C102	0.75000	0.58289	0.08289
C103	0.75000	0.61769	0.11769
C104	0.76707	0.61051	0.15902
H105	0.77940	0.58310	0.16510
C106	0.76685	0.64162	0.19154
H107	0.77800	0.63500	0.21930
C108	0.75000	0.68284	0.18284
C109	0.75000	0.71702	0.21702
C110	0.71789	0.75000	0.21789
H111	0.69620	0.75000	0.19620
O112	0.84961	0.50000	0.03703
Zn13	0.94806	0.21258	0.50000
O114	0.00000	0.25000	0.50000
O115	0.91182	0.22472	0.55094
C116	0.91711	0.25000	0.58289
C117	0.88231	0.25000	0.61769
C118	0.84098	0.23293	0.61051
H119	0.83490	0.22060	0.58310
C120	0.80846	0.23315	0.64162
H121	0.78070	0.22200	0.63500
C122	0.81716	0.25000	0.68284

C123	0.78298	0.25000	0.71702
C124	0.78211	0.28211	0.75000
H125	0.80380	0.30380	0.75000
O126	0.96297	0.15039	0.50000
C127	0.00000	0.13094	0.50000
Zn28	0.05194	0.21258	0.50000
O129	0.08818	0.22472	0.44906
C130	0.08289	0.25000	0.41711
C131	0.11769	0.25000	0.38231
C132	0.15902	0.23293	0.38949
H133	0.16510	0.22060	0.41690
C134	0.19154	0.23315	0.35838
H135	0.21930	0.22200	0.36500
C136	0.18284	0.25000	0.31716
C137	0.21702	0.25000	0.28298
C138	0.21789	0.28211	0.25000
H139	0.19620	0.30380	0.25000
O140	0.03703	0.15039	0.50000
Zn41	0.94806	0.78742	0.50000
O142	0.00000	0.75000	0.50000
O143	0.91182	0.77528	0.44906
C144	0.91711	0.75000	0.41711
C145	0.88231	0.75000	0.38231
C146	0.84098	0.76707	0.38949
H147	0.83490	0.77940	0.41690
C148	0.80846	0.76685	0.35838
H149	0.78070	0.77800	0.36500
C150	0.81716	0.75000	0.31716
C151	0.78298	0.75000	0.28298
C152	0.78211	0.71789	0.25000
H153	0.80380	0.69620	0.25000
O154	0.96297	0.84961	0.50000
C155	0.00000	0.86906	0.50000
Zn56	0.05194	0.78742	0.50000
O157	0.08818	0.77528	0.55094
C158	0.08289	0.75000	0.58289
C159	0.11769	0.75000	0.61769
C160	0.15902	0.76707	0.61051
H161	0.16510	0.77940	0.58310
C162	0.19154	0.76685	0.64162
H163	0.21930	0.77800	0.63500
C164	0.18284	0.75000	0.68284
C165	0.21702	0.75000	0.71702
C166	0.21789	0.71789	0.75000
H167	0.19620	0.69620	0.75000

O168	0.03703	0.84961	0.50000
Zn69	0.44806	0.00000	0.28742
O170	0.41182	0.05094	0.27528
C171	0.34098	0.11051	0.26707
H172	0.33490	0.08310	0.27940
C173	0.30846	0.14162	0.26685
H174	0.28070	0.13500	0.27800
O175	0.46297	0.00000	0.34961
C176	0.50000	0.00000	0.36906
Zn77	0.55194	0.00000	0.28742
O178	0.58818	0.94906	0.27528
C179	0.65902	0.88949	0.26707
H180	0.66510	0.91690	0.27940
C181	0.69154	0.85838	0.26685
H182	0.71930	0.86500	0.27800
O183	0.53703	0.00000	0.34961
Zn84	0.44806	0.00000	0.71258
O185	0.41182	0.94906	0.72472
C186	0.34098	0.88949	0.73293
H187	0.33490	0.91690	0.72060
C188	0.30846	0.85838	0.73315
H189	0.28070	0.86500	0.72200
O190	0.46297	0.00000	0.65039
C191	0.50000	0.00000	0.63094
Zn92	0.55194	0.00000	0.71258
O193	0.58818	0.05094	0.72472
C194	0.65902	0.11051	0.73293
H195	0.66510	0.08310	0.72060
C196	0.69154	0.14162	0.73315
H197	0.71930	0.13500	0.72200
O198	0.53703	0.00000	0.65039
Zn99	0.00000	0.71258	0.55194
O200	0.05094	0.72472	0.58818
C201	0.11051	0.73293	0.65902
H202	0.08310	0.72060	0.66510
C203	0.14162	0.73315	0.69154
H204	0.13500	0.72200	0.71930
O205	0.00000	0.65039	0.53703
C206	0.00000	0.63094	0.50000
Zn7	0.00000	0.71258	0.44806
O208	0.94906	0.72472	0.41182
C209	0.88949	0.73293	0.34098
H210	0.91690	0.72060	0.33490
C211	0.85838	0.73315	0.30846
H212	0.86500	0.72200	0.28070

O213	0.00000	0.65039	0.46297
Zn14	0.00000	0.28742	0.55194
O215	0.94906	0.27528	0.58818
C216	0.88949	0.26707	0.65902
H217	0.91690	0.27940	0.66510
C218	0.85838	0.26685	0.69154
H219	0.86500	0.27800	0.71930
O220	0.00000	0.34961	0.53703
C221	0.00000	0.36906	0.50000
Zn22	0.00000	0.28742	0.44806
O223	0.05094	0.27528	0.41182
C224	0.11051	0.26707	0.34098
H225	0.08310	0.27940	0.33490
C226	0.14162	0.26685	0.30846
H227	0.13500	0.27800	0.28070
O228	0.00000	0.34961	0.46297
Zn29	0.71258	0.44806	0.00000
O230	0.72472	0.41182	0.94906
C231	0.73293	0.34098	0.88949
H232	0.72060	0.33490	0.91690
C233	0.73315	0.30846	0.85838
H234	0.72200	0.28070	0.86500
O235	0.65039	0.46297	0.00000
C236	0.63094	0.50000	0.00000
Zn37	0.71258	0.55194	0.00000
O238	0.72472	0.58818	0.05094
C239	0.73293	0.65902	0.11051
H240	0.72060	0.66510	0.08310
C241	0.73315	0.69154	0.14162
H242	0.72200	0.71930	0.13500
O243	0.65039	0.53703	0.00000
Zn44	0.28742	0.44806	0.00000
O245	0.27528	0.41182	0.05094
C246	0.26707	0.34098	0.11051
H247	0.27940	0.33490	0.08310
C248	0.26685	0.30846	0.14162
H249	0.27800	0.28070	0.13500
O250	0.34961	0.46297	0.00000
C251	0.36906	0.50000	0.00000
Zn52	0.28742	0.55194	0.00000
O253	0.27528	0.58818	0.94906
C254	0.26707	0.65902	0.88949
H255	0.27940	0.66510	0.91690
C256	0.26685	0.69154	0.85838
H257	0.27800	0.71930	0.86500

O258	0.34961	0.53703	0.00000
O259	0.44906	0.08818	0.77528
C260	0.41711	0.08289	0.75000
C261	0.38231	0.11769	0.75000
C262	0.38949	0.15902	0.76707
H263	0.41690	0.16510	0.77940
C264	0.35838	0.19154	0.76685
H265	0.36500	0.21930	0.77800
C266	0.31716	0.18284	0.75000
C267	0.28298	0.21702	0.75000
C268	0.25000	0.21789	0.71789
H269	0.25000	0.19620	0.69620
O270	0.55094	0.91182	0.77528
C271	0.58289	0.91711	0.75000
C272	0.61769	0.88231	0.75000
C273	0.61051	0.84098	0.76707
H274	0.58310	0.83490	0.77940
C275	0.64162	0.80846	0.76685
H276	0.63500	0.78070	0.77800
C277	0.68284	0.81716	0.75000
C278	0.71702	0.78298	0.75000
C279	0.75000	0.78211	0.71789
H280	0.75000	0.80380	0.69620
O281	0.55094	0.08818	0.22472
C282	0.58289	0.08289	0.25000
C283	0.61769	0.11769	0.25000
C284	0.61051	0.15902	0.23293
H285	0.58310	0.16510	0.22060
C286	0.64162	0.19154	0.23315
H287	0.63500	0.21930	0.22200
C288	0.68284	0.18284	0.25000
C289	0.71702	0.21702	0.25000
C290	0.75000	0.21789	0.28211
H291	0.75000	0.19620	0.30380
O292	0.44906	0.91182	0.22472
C293	0.41711	0.91711	0.25000
C294	0.38231	0.88231	0.25000
C295	0.38949	0.84098	0.23293
H296	0.41690	0.83490	0.22060
C297	0.35838	0.80846	0.23315
H298	0.36500	0.78070	0.22200
C299	0.31716	0.81716	0.25000
C300	0.28298	0.78298	0.25000
C301	0.25000	0.78211	0.28211
H302	0.25000	0.80380	0.30380

O303	0.77528	0.44906	0.08818
C304	0.75000	0.41711	0.08289
C305	0.75000	0.38231	0.11769
C306	0.76707	0.38949	0.15902
H307	0.77940	0.41690	0.16510
C308	0.76685	0.35838	0.19154
H309	0.77800	0.36500	0.21930
C310	0.75000	0.31716	0.18284
C311	0.75000	0.28298	0.21702
C312	0.71789	0.25000	0.21789
H313	0.69620	0.25000	0.19620
O314	0.77528	0.55094	0.91182
C315	0.75000	0.58289	0.91711
C316	0.75000	0.61769	0.88231
C317	0.76707	0.61051	0.84098
H318	0.77940	0.58310	0.83490
C319	0.76685	0.64162	0.80846
H320	0.77800	0.63500	0.78070
C321	0.75000	0.68284	0.81716
C322	0.75000	0.71702	0.78298
C323	0.71789	0.75000	0.78211
H324	0.69620	0.75000	0.80380
O325	0.22472	0.55094	0.08818
C326	0.25000	0.58289	0.08289
C327	0.25000	0.61769	0.11769
C328	0.23293	0.61051	0.15902
H329	0.22060	0.58310	0.16510
C330	0.23315	0.64162	0.19154
H331	0.22200	0.63500	0.21930
C332	0.25000	0.68284	0.18284
C333	0.25000	0.71702	0.21702
C334	0.28211	0.75000	0.21789
H335	0.30380	0.75000	0.19620
O336	0.22472	0.44906	0.91182
C337	0.25000	0.41711	0.91711
C338	0.25000	0.38231	0.88231
C339	0.23293	0.38949	0.84098
H340	0.22060	0.41690	0.83490
C341	0.23315	0.35838	0.80846
H342	0.22200	0.36500	0.78070
C343	0.25000	0.31716	0.81716
C344	0.25000	0.28298	0.78298
C345	0.28211	0.25000	0.78211
H346	0.30380	0.25000	0.80380
O347	0.08818	0.77528	0.44906

C348	0.08289	0.75000	0.41711
C349	0.11769	0.75000	0.38231
C350	0.15902	0.76707	0.38949
H351	0.16510	0.77940	0.41690
C352	0.19154	0.76685	0.35838
H353	0.21930	0.77800	0.36500
C354	0.18284	0.75000	0.31716
C355	0.21702	0.75000	0.28298
C356	0.21789	0.71789	0.25000
H357	0.19620	0.69620	0.25000
O358	0.91182	0.77528	0.55094
C359	0.91711	0.75000	0.58289
C360	0.88231	0.75000	0.61769
C361	0.84098	0.76707	0.61051
H362	0.83490	0.77940	0.58310
C363	0.80846	0.76685	0.64162
H364	0.78070	0.77800	0.63500
C365	0.81716	0.75000	0.68284
C366	0.78298	0.75000	0.71702
C367	0.78211	0.71789	0.75000
H368	0.80380	0.69620	0.75000
O369	0.08818	0.22472	0.55094
C370	0.08289	0.25000	0.58289
C371	0.11769	0.25000	0.61769
C372	0.15902	0.23293	0.61051
H373	0.16510	0.22060	0.58310
C374	0.19154	0.23315	0.64162
H375	0.21930	0.22200	0.63500
C376	0.18284	0.25000	0.68284
C377	0.21702	0.25000	0.71702
C378	0.21789	0.28211	0.75000
H379	0.19620	0.30380	0.75000
O380	0.91182	0.22472	0.44906
C381	0.91711	0.25000	0.41711
C382	0.88231	0.25000	0.38231
C383	0.84098	0.23293	0.38949
H384	0.83490	0.22060	0.41690
C385	0.80846	0.23315	0.35838
H386	0.78070	0.22200	0.36500
C387	0.81716	0.25000	0.31716
C388	0.78298	0.25000	0.28298
C389	0.78211	0.28211	0.25000
H390	0.80380	0.30380	0.25000
O391	0.58818	0.94906	0.72472
C392	0.65902	0.88949	0.73293

H393	0.66510	0.91690	0.72060
C394	0.69154	0.85838	0.73315
H395	0.71930	0.86500	0.72200
O396	0.41182	0.05094	0.72472
C397	0.34098	0.11051	0.73293
H398	0.33490	0.08310	0.72060
C399	0.30846	0.14162	0.73315
H400	0.28070	0.13500	0.72200
O401	0.58818	0.05094	0.27528
C402	0.65902	0.11051	0.26707
H403	0.66510	0.08310	0.27940
C404	0.69154	0.14162	0.26685
H405	0.71930	0.13500	0.27800
O406	0.41182	0.94906	0.27528
C407	0.34098	0.88949	0.26707
H408	0.33490	0.91690	0.27940
C409	0.30846	0.85838	0.26685
H410	0.28070	0.86500	0.27800
O411	0.94906	0.27528	0.41182
C412	0.88949	0.26707	0.34098
H413	0.91690	0.27940	0.33490
C414	0.85838	0.26685	0.30846
H415	0.86500	0.27800	0.28070
O416	0.05094	0.27528	0.58818
C417	0.11051	0.26707	0.65902
H418	0.08310	0.27940	0.66510
C419	0.14162	0.26685	0.69154
H420	0.13500	0.27800	0.71930
O421	0.05094	0.72472	0.41182
C422	0.11051	0.73293	0.34098
H423	0.08310	0.72060	0.33490
C424	0.14162	0.73315	0.30846
H425	0.13500	0.72200	0.28070
O426	0.94906	0.72472	0.58818
C427	0.88949	0.73293	0.65902
H428	0.91690	0.72060	0.66510
C429	0.85838	0.73315	0.69154
H430	0.86500	0.72200	0.71930
O431	0.27528	0.58818	0.05094
C432	0.26707	0.65902	0.11051
H433	0.27940	0.66510	0.08310
C434	0.26685	0.69154	0.14162
H435	0.27800	0.71930	0.13500
O436	0.27528	0.41182	0.94906
C437	0.26707	0.34098	0.88949

H438	0.27940	0.33490	0.91690
C439	0.26685	0.30846	0.85838
H440	0.27800	0.28070	0.86500
O441	0.72472	0.58818	0.94906
C442	0.73293	0.65902	0.88949
H443	0.72060	0.66510	0.91690
C444	0.73315	0.69154	0.85838
H445	0.72200	0.71930	0.86500
O446	0.72472	0.41182	0.05094
C447	0.73293	0.34098	0.11051
H448	0.72060	0.33490	0.08310
C449	0.73315	0.30846	0.14162
H450	0.72200	0.28070	0.13500
C451	0.47781	1.00000	0.50772
C452	0.52219	1.00000	0.49228
C453	0.55716	1.00000	0.52304
H454	0.58923	1.00000	0.51264
C455	0.54835	1.00000	0.56853
H456	0.57380	1.00000	0.59060
C457	0.50461	1.00000	0.58374
C458	0.46948	1.00000	0.55354
H459	0.43787	1.00000	0.56528
C460	0.53052	1.00000	0.44646
H461	0.56213	1.00000	0.43472
C462	0.49539	1.00000	0.41626
C463	0.45165	1.00000	0.43147
H464	0.42620	1.00000	0.40940
C465	0.44284	1.00000	0.47696
H466	0.41077	1.00000	0.48736
C467	0.50712	0.52239	1.00000
C468	0.49288	0.47761	1.00000
C469	0.52456	0.44348	1.00000
H470	0.51501	0.41114	1.00000
C471	0.56980	0.45349	1.00000
H472	0.59254	0.42864	1.00000
C473	0.58384	0.49762	1.00000
C474	0.55271	0.53194	1.00000
H475	0.56360	0.56385	1.00000
C476	0.44729	0.46806	1.00000
H477	0.43640	0.43615	1.00000
C478	0.41616	0.50238	1.00000
C479	0.43020	0.54651	1.00000
H480	0.40746	0.57136	1.00000
C481	0.47544	0.55652	1.00000
H482	0.48499	0.58886	1.00000

C483	1.00000	0.49288	0.52239
C484	1.00000	0.50712	0.47761
C485	1.00000	0.47544	0.44348
H486	1.00000	0.48499	0.41114
C487	1.00000	0.43020	0.45349
H488	1.00000	0.40746	0.42864
C489	1.00000	0.41616	0.49762
C490	1.00000	0.44729	0.53194
H491	1.00000	0.43640	0.56385
C492	1.00000	0.55271	0.46806
H493	1.00000	0.56360	0.43615
C494	1.00000	0.58384	0.50238
C495	1.00000	0.56980	0.54651
H496	1.00000	0.59254	0.57136
C497	1.00000	0.52456	0.55652
H498	1.00000	0.51501	0.58886
C499	1.02239	0.99288	0.50000
C500	0.97761	1.00712	0.50000
C501	0.94348	0.97544	0.50000
H502	0.91114	0.98499	0.50000
C503	0.95349	0.93020	0.50000
H504	0.92864	0.90746	0.50000
C505	0.99762	0.91616	0.50000
C506	1.03194	0.94729	0.50000
H507	1.06385	0.93640	0.50000
C508	0.96806	1.05271	0.50000
H509	0.93615	1.06360	0.50000
C510	1.00238	1.08384	0.50000
C511	1.04651	1.06980	0.50000
H512	1.07136	1.09254	0.50000
C513	1.05652	1.02456	0.50000
H514	1.08886	1.01501	0.50000
C515	0.99169	0.50000	0.97803
C516	1.00831	0.50000	1.02197
C517	0.97851	0.50000	1.05776
H518	0.98978	0.50000	1.08954
C519	0.93280	0.50000	1.05018
H520	0.91143	0.50000	1.07623
C521	0.91641	0.50000	1.00688
C522	0.94566	0.50000	0.97094
H523	0.93306	0.50000	0.93965
C524	1.05434	0.50000	1.02906
H525	1.06694	0.50000	1.06035
C526	1.08359	0.50000	0.99312
C527	1.06720	0.50000	0.94982

H528	1.08857	0.50000	0.92377
C529	1.02149	0.50000	0.94224
H530	1.01022	0.50000	0.91046
C531	0.50000	1.02197	0.99169
C532	0.50000	0.97803	1.00831
C533	0.50000	0.94224	0.97851
H534	0.50000	0.91046	0.98978
C535	0.50000	0.94982	0.93280
H536	0.50000	0.92377	0.91143
C537	0.50000	0.99312	0.91641
C538	0.50000	1.02906	0.94566
H539	0.50000	1.06035	0.93306
C540	0.50000	0.97094	1.05434
H541	0.50000	0.93965	1.06694
C542	0.50000	1.00688	1.08359
C543	0.50000	1.05018	1.06720
H544	0.50000	1.07623	1.08857
C545	0.50000	1.05776	1.02149
H546	0.50000	1.08954	1.01022
Li47	0.62852	0.81779	0.33079
Li48	0.80129	0.80129	0.19871
Li49	0.37148	0.18221	0.33079
Li50	0.19871	0.19871	0.19871
Li51	0.37148	0.81779	0.66921
Li52	0.19871	0.80129	0.80129
Li53	0.62852	0.18221	0.66921
Li54	0.80129	0.19871	0.80129
Li55	0.33079	0.62852	0.81779
Li56	0.33079	0.37148	0.18221
Li57	0.66921	0.37148	0.81779
Li58	0.66921	0.62852	0.18221
Li59	0.81779	0.33079	0.62852
Li60	0.18221	0.33079	0.37148
Li61	0.81779	0.66921	0.37148
Li62	0.18221	0.66921	0.62852
Li63	0.37148	0.18221	0.66921
Li64	0.19871	0.19871	0.80129
Li65	0.62852	0.81779	0.66921
Li66	0.80129	0.80129	0.80129
Li67	0.62852	0.18221	0.33079
Li68	0.80129	0.19871	0.19871
Li69	0.37148	0.81779	0.33079
Li70	0.19871	0.80129	0.19871
Li71	0.66921	0.37148	0.18221
Li72	0.66921	0.62852	0.81779

Li73	0.33079	0.62852	0.18221
Li74	0.33079	0.37148	0.81779
Li75	0.18221	0.66921	0.37148
Li76	0.81779	0.66921	0.62852
Li77	0.18221	0.33079	0.62852
Li78	0.81779	0.33079	0.37148
Li79	0.53278	0.48957	0.91152
Li80	0.46722	0.51043	1.08848
Li81	1.08848	0.46722	0.48957
Li82	0.91152	0.53278	0.51043
Li83	0.51130	1.08848	0.53249
Li84	0.48870	0.91152	0.46751
Li85	0.98957	0.96722	0.58848
Li86	1.01043	1.03278	0.41152
Li87	1.03217	0.41152	0.98783
Li88	0.96783	0.58848	1.01217
Li89	0.58848	0.98783	0.96783
Li90	0.41152	1.01217	1.03217

9 Numerical Data

9.1 COF102

Table 1: Qst

Pres	COF102		COF102-1Li		COF102-Na		COF102-K	
Bar	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol
1.0	1.065	4.458	4.699	19.659	3.129	13.093	2.166	9.062
2.0	1.065	4.458	4.624	19.347	3.129	13.093	2.165	9.057
3.0	1.067	4.466	4.663	19.512	3.128	13.089	2.164	9.054
4.0	1.067	4.465	4.646	19.439	3.124	13.070	2.163	9.050
5.0	1.068	4.469	4.630	19.373	3.118	13.046	2.163	9.049
10.0	1.067	4.464	4.558	19.069	3.107	12.999	2.157	9.024
20.0	1.070	4.478	4.435	18.556	3.083	12.899	2.155	9.018
30.0	1.070	4.477	4.347	18.187	3.053	12.772	2.148	8.988
40.0	1.071	4.481	4.273	17.876	3.029	12.672	2.143	8.967
50.0	1.071	4.481	4.206	17.599	3.011	12.599	2.143	8.967
60.0	1.070	4.477	4.156	17.388	2.985	12.490	2.141	8.957
70.0	1.071	4.480	4.095	17.134	2.967	12.416	2.133	8.925
80.0	1.072	4.484	4.058	16.981	2.957	12.371	2.131	8.918
90.0	1.071	4.483	3.989	16.688	2.939	12.296	2.123	8.884
100.0	1.072	4.485	3.970	16.609	2.922	12.225	2.123	8.882

Table 2: Total uptake

Pres	COF102			COF102-1Li			COF102-Na			COF102-K		
	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot
	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L
Bar												
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.0	0.916	0.036	0.153	21.848	0.807	3.553	6.039	0.196	0.982	2.576	0.075	0.419
2.0	1.446	0.057	0.241	36.766	1.350	5.978	11.681	0.379	1.899	4.802	0.139	0.781
3.0	1.931	0.077	0.322	47.371	1.732	7.703	17.029	0.552	2.769	7.095	0.205	1.154
4.0	2.431	0.096	0.405	56.477	2.059	9.183	21.816	0.706	3.547	9.341	0.270	1.519
5.0	2.938	0.116	0.490	63.090	2.294	10.258	26.394	0.853	4.292	11.517	0.332	1.873
10.0	5.611	0.222	0.936	86.094	3.105	13.999	46.249	1.485	7.520	21.801	0.627	3.545
20.0	10.899	0.430	1.818	108.889	3.895	17.705	74.512	2.370	12.116	39.457	1.130	6.416
30.0	15.997	0.630	2.668	123.264	4.386	20.043	94.145	2.976	15.308	54.191	1.545	8.812
40.0	20.858	0.820	3.479	133.750	4.742	21.748	108.890	3.426	17.706	66.747	1.897	10.853
50.0	25.487	1.001	4.251	141.569	5.005	23.019	121.324	3.803	19.727	78.002	2.209	12.683
60.0	29.941	1.173	4.994	148.296	5.230	24.113	130.841	4.089	21.275	87.698	2.477	14.260
70.0	34.166	1.337	5.698	153.873	5.417	25.020	139.173	4.338	22.630	95.967	2.704	15.604
80.0	38.272	1.495	6.383	159.793	5.613	25.983	146.851	4.566	23.878	103.934	2.922	16.900
90.0	42.188	1.645	7.036	164.142	5.757	26.690	153.764	4.771	25.002	110.757	3.108	18.009
100.0	45.990	1.791	7.670	168.086	5.887	27.331	159.115	4.929	25.872	117.464	3.290	19.100

9.2 COF103

Table 3: Qst

Pres	COF103		COF103-1Li		COF103-Na		COF103-K	
Bar	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol
1.0	1.040	4.351	4.797	20.069	3.158	13.213	2.042	8.545
2.0	1.040	4.352	4.771	19.963	3.157	13.208	2.042	8.542
3.0	1.042	4.360	4.754	19.891	3.153	13.194	2.040	8.535
4.0	1.039	4.346	4.732	19.798	3.152	13.186	2.040	8.534
5.0	1.040	4.351	4.711	19.709	3.127	13.081	2.039	8.532
10.0	1.042	4.360	4.639	19.409	3.097	12.960	2.036	8.520
20.0	1.019	4.265	4.496	18.809	3.082	12.896	2.029	8.489
30.0	1.042	4.360	4.398	18.400	3.035	12.699	2.028	8.487
40.0	1.041	4.356	4.325	18.095	3.020	12.637	2.028	8.484
50.0	1.043	4.363	4.232	17.706	2.985	12.490	2.018	8.442
60.0	1.042	4.360	4.155	17.383	2.955	12.362	2.017	8.437
70.0	1.041	4.357	4.096	17.138	2.935	12.281	2.013	8.421
80.0	1.044	4.370	4.049	16.941	2.915	12.198	2.007	8.396
90.0	1.044	4.369	3.995	16.716	2.894	12.110	2.006	8.394
100.0	1.044	4.366	3.947	16.512	2.876	12.032	2.002	8.376

Table 4: Total Uptake

Pres	COF103			COF103-1Li			COF103-Na			COF103-K		
	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot
	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L
Bar												
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.0	0.997	0.038	0.145	22.791	0.812	3.312	5.972	0.188	0.868	2.394	0.067	0.348
2.0	1.584	0.060	0.230	37.502	1.330	5.450	11.583	0.365	1.683	4.446	0.125	0.646
3.0	2.152	0.082	0.313	48.752	1.722	7.084	16.770	0.527	2.437	6.551	0.184	0.952
4.0	2.717	0.104	0.395	56.755	1.999	8.247	21.659	0.680	3.147	8.649	0.243	1.257
5.0	3.324	0.127	0.483	63.615	2.235	9.244	26.483	0.830	3.848	10.752	0.302	1.562
10.0	6.400	0.244	0.930	86.460	3.013	12.564	46.185	1.438	6.711	20.495	0.574	2.978
20.0	12.479	0.475	1.813	109.634	3.791	15.932	73.976	2.284	10.749	37.881	1.056	5.504
30.0	18.299	0.694	2.659	124.496	4.282	18.091	93.213	2.861	13.545	52.988	1.471	7.700
40.0	23.767	0.900	3.454	134.728	4.618	19.578	109.571	3.346	15.922	66.350	1.836	9.641
50.0	29.104	1.100	4.229	142.886	4.884	20.764	121.707	3.703	17.685	77.227	2.130	11.222
60.0	34.277	1.293	4.981	149.754	5.107	21.762	131.698	3.995	19.137	87.728	2.413	12.748
70.0	39.104	1.472	5.682	156.400	5.321	22.727	141.111	4.269	20.505	97.578	2.676	14.179
80.0	43.924	1.650	6.383	162.071	5.504	23.552	149.466	4.510	21.719	105.712	2.893	15.361
90.0	48.472	1.818	7.044	167.403	5.675	24.326	155.838	4.693	22.645	113.308	3.094	16.465
100.0	52.937	1.982	7.693	172.283	5.830	25.036	162.632	4.888	23.632	120.810	3.293	17.555

9.3 COF202

Table 5: Qst

Pres	COF202		COF202-1Li		COF202-Na		COF202-K	
Bar	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol
1.0	1.075	4.500	4.696	19.647	3.140	13.137	2.130	8.912
2.0	1.073	4.489	4.675	19.561	3.127	13.082	2.127	8.901
3.0	1.073	4.490	4.657	19.485	3.124	13.072	2.125	8.891
4.0	1.075	4.497	4.631	19.376	3.116	13.037	2.125	8.890
5.0	1.074	4.493	4.617	19.315	3.110	13.014	2.123	8.884
10.0	1.023	4.280	4.528	18.943	3.082	12.893	2.118	8.862
20.0	1.074	4.492	4.402	18.418	3.039	12.717	2.109	8.822
30.0	1.070	4.476	4.282	17.917	3.005	12.574	2.098	8.778
40.0	1.072	4.484	4.193	17.543	2.974	12.441	2.092	8.755
50.0	1.071	4.481	4.122	17.245	2.941	12.305	2.086	8.726
60.0	1.070	4.478	4.049	16.943	2.921	12.220	2.073	8.674
70.0	1.050	4.392	3.989	16.691	2.890	12.092	2.066	8.642
80.0	1.069	4.471	3.920	16.400	2.869	12.004	2.063	8.633
90.0	1.068	4.470	3.904	16.336	2.849	11.919	2.055	8.596
100.0	1.068	4.469	3.847	16.098	2.838	11.874	2.049	8.574

Table 6: Total Uptake

Pres	COF202			COF202-1Li			COF202-Na			COF202-K		
	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot
	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L
Bar												
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.0	0.952	0.022	0.117	20.564	0.466	2.523	5.485	0.115	0.673	2.281	0.044	0.280
2.0	1.506	0.036	0.185	34.296	0.774	4.208	10.461	0.218	1.284	4.214	0.082	0.517
3.0	2.025	0.048	0.249	44.667	1.006	5.480	15.287	0.319	1.876	6.182	0.120	0.759
4.0	2.554	0.060	0.313	51.814	1.165	6.357	19.751	0.412	2.423	8.219	0.159	1.008
5.0	3.096	0.073	0.380	58.727	1.318	7.205	23.957	0.499	2.939	10.094	0.195	1.238
10.0	5.981	0.141	0.734	79.693	1.780	9.778	41.627	0.864	5.107	19.204	0.371	2.356
20.0	11.566	0.273	1.419	101.951	2.266	12.509	66.734	1.377	8.188	35.286	0.679	4.329
30.0	16.978	0.400	2.083	115.144	2.552	14.127	85.519	1.758	10.493	48.967	0.940	6.008
40.0	22.118	0.520	2.714	125.760	2.781	15.430	99.624	2.042	12.223	60.959	1.167	7.479
50.0	27.028	0.635	3.316	134.101	2.960	16.453	110.958	2.269	13.614	71.711	1.370	8.798
60.0	31.693	0.743	3.888	141.129	3.110	17.316	121.180	2.473	14.868	80.749	1.540	9.907
70.0	36.588	0.857	4.489	146.979	3.235	18.033	129.156	2.632	15.846	89.194	1.699	10.944
80.0	40.667	0.952	4.990	153.322	3.370	18.811	136.022	2.768	16.689	97.204	1.848	11.926
90.0	44.864	1.049	5.504	158.570	3.481	19.455	143.116	2.908	17.559	104.485	1.984	12.820
100.0	49.088	1.147	6.023	162.813	3.571	19.976	149.365	3.031	18.326	110.765	2.101	13.590

9.4 MOF177

Table 7: Qst

Pres	MOF177		MOF177-1Li		MOF177-Na		MOF177-K	
Bar	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol
1.0	1.167	4.881	5.007	20.949	3.986	16.678	2.253	9.426
2.0	1.168	4.887	4.900	20.501	3.834	16.042	2.251	9.416
3.0	1.168	4.888	4.841	20.255	3.740	15.650	2.240	9.373
4.0	1.168	4.886	4.795	20.061	3.657	15.302	2.235	9.350
5.0	1.169	4.892	4.763	19.928	3.602	15.071	2.223	9.301
10.0	1.171	4.897	4.631	19.377	3.421	14.314	2.200	9.203
20.0	1.173	4.909	4.460	18.659	3.238	13.546	2.161	9.044
30.0	1.176	4.920	4.315	18.055	3.172	13.270	2.135	8.933
40.0	1.179	4.934	4.215	17.637	3.103	12.985	2.115	8.849
50.0	1.180	4.936	4.123	17.249	3.055	12.780	2.093	8.759
60.0	1.184	4.952	4.041	16.908	3.006	12.577	2.079	8.699
70.0	1.184	4.952	3.970	16.609	2.974	12.443	2.063	8.631
80.0	1.189	4.976	3.908	16.352	2.934	12.278	2.051	8.582
90.0	1.192	4.986	3.847	16.096	2.909	12.170	2.043	8.547
100.0	1.194	4.994	3.803	15.912	2.882	12.060	2.034	8.511

Table 8: Total Uptake

Pres	MOF177			MOF177-1Li			MOF177-Na			MOF177-K		
	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot
Bar	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.0	1.488	0.033	0.139	38.365	0.797	3.593	14.332	0.270	1.342	3.998	0.069	0.374
2.0	2.532	0.056	0.237	59.854	1.237	5.605	24.601	0.463	2.304	7.793	0.134	0.730
3.0	3.616	0.079	0.339	74.858	1.543	7.011	33.317	0.626	3.120	11.476	0.198	1.075
4.0	4.759	0.104	0.446	86.178	1.772	8.071	40.932	0.768	3.833	15.042	0.259	1.409
5.0	5.906	0.129	0.553	96.125	1.972	9.002	47.931	0.898	4.489	18.533	0.319	1.736
10.0	11.707	0.256	1.096	126.334	2.576	11.832	76.062	1.418	7.123	34.507	0.592	3.232
20.0	23.091	0.504	2.163	160.327	3.247	15.015	114.953	2.128	10.766	61.531	1.050	5.763
30.0	34.129	0.743	3.196	179.995	3.631	16.857	142.291	2.621	13.326	84.080	1.429	7.874
40.0	44.868	0.975	4.202	196.046	3.942	18.360	163.546	3.000	15.317	104.019	1.762	9.742
50.0	54.946	1.191	5.146	208.170	4.175	19.496	182.252	3.332	17.069	120.322	2.033	11.269
60.0	65.036	1.407	6.091	219.341	4.389	20.542	197.230	3.596	18.471	135.550	2.284	12.695
70.0	74.665	1.612	6.993	228.887	4.572	21.436	209.998	3.820	19.667	149.262	2.509	13.979
80.0	84.219	1.814	7.887	237.851	4.742	22.276	221.706	4.024	20.764	161.513	2.710	15.126
90.0	93.497	2.010	8.756	244.955	4.877	22.941	233.306	4.226	21.850	173.268	2.901	16.227
100.0	102.386	2.197	9.589	253.704	5.042	23.760	242.496	4.385	22.711	183.144	3.062	17.152

9.5 MOF180

Table 9: Qst

Pres	MOF180		MOF180-1Li		MOF180-Na		MOF180-K	
Bar	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol
1.0	0.880	3.682	4.750	19.872	3.855	16.128	1.754	7.340
2.0	0.878	3.675	4.655	19.478	3.627	15.177	1.745	7.302
3.0	0.865	3.618	4.585	19.185	3.473	14.530	1.739	7.276
4.0	0.832	3.479	4.534	18.972	3.360	14.059	1.731	7.243
5.0	0.833	3.484	4.479	18.739	3.283	13.737	1.731	7.242
10.0	0.837	3.500	4.277	17.895	3.045	12.739	1.709	7.150
20.0	0.840	3.514	4.014	16.793	2.832	11.851	1.677	7.016
30.0	0.845	3.536	3.792	15.865	2.707	11.326	1.654	6.918
40.0	0.847	3.545	3.634	15.204	2.622	10.972	1.639	6.858
50.0	0.853	3.570	3.495	14.623	2.538	10.620	1.616	6.761
60.0	0.863	3.611	3.384	14.158	2.484	10.394	1.602	6.703
70.0	0.877	3.668	3.272	13.689	2.434	10.182	1.589	6.646
80.0	0.880	3.682	3.181	13.311	2.388	9.992	1.572	6.578
90.0	0.879	3.677	3.111	13.017	2.343	9.801	1.567	6.556
100.0	0.878	3.674	3.053	12.773	2.312	9.672	1.556	6.511

Table 10: Total Uptake

Pres	MOF180			MOF180-1Li			MOF180-Na			MOF180-K		
	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot
Bar	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.0	2.079	0.041	0.103	36.700	0.681	1.819	14.485	0.247	0.718	4.249	0.067	0.211
2.0	3.775	0.074	0.187	58.636	1.084	2.906	24.806	0.422	1.229	8.371	0.131	0.415
3.0	5.492	0.107	0.272	74.582	1.375	3.696	33.405	0.567	1.656	12.369	0.194	0.613
4.0	7.026	0.137	0.348	87.145	1.603	4.319	41.584	0.705	2.061	16.319	0.256	0.809
5.0	8.755	0.170	0.434	97.071	1.782	4.811	49.026	0.830	2.430	20.220	0.316	1.002
10.0	17.280	0.336	0.856	131.568	2.400	6.520	80.354	1.353	3.982	38.834	0.606	1.925
20.0	33.969	0.658	1.684	174.138	3.153	8.630	127.465	2.129	6.317	72.525	1.126	3.594
30.0	50.248	0.970	2.490	202.472	3.647	10.034	163.671	2.718	8.111	102.389	1.582	5.074
40.0	65.898	1.268	3.266	226.127	4.056	11.207	195.303	3.226	9.679	130.041	2.000	6.445
50.0	81.303	1.560	4.029	246.506	4.405	12.217	219.878	3.617	10.897	153.844	2.358	7.624
60.0	97.262	1.861	4.820	265.312	4.725	13.149	242.811	3.979	12.034	176.918	2.702	8.768
70.0	113.321	2.162	5.616	281.988	5.007	13.975	263.678	4.306	13.068	197.797	3.011	9.803
80.0	127.269	2.421	6.307	298.295	5.281	14.783	283.961	4.622	14.073	217.695	3.304	10.789
90.0	141.119	2.678	6.994	313.359	5.533	15.530	299.226	4.859	14.829	236.820	3.584	11.737
100.0	154.262	2.920	7.645	327.605	5.770	16.236	316.849	5.130	15.703	253.936	3.833	12.585

9.6 MOF200

Table 11: Qst

Pres	MOF200		MOF200-1Li		MOF200-Na		MOF200-K	
Bar	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol
1.0	0.859	3.594	4.773	19.971	3.394	14.202	1.972	8.253
2.0	0.860	3.596	4.701	19.669	3.298	13.799	1.966	8.225
3.0	0.847	3.542	4.655	19.478	3.237	13.543	1.946	8.143
4.0	0.823	3.443	4.610	19.290	3.184	13.323	1.942	8.125
5.0	0.822	3.439	4.583	19.176	3.158	13.212	1.939	8.111
10.0	0.822	3.441	4.421	18.498	3.037	12.706	1.915	8.011
20.0	0.824	3.446	4.181	17.492	2.913	12.188	1.861	7.787
30.0	0.822	3.439	4.016	16.802	2.814	11.772	1.821	7.618
40.0	0.825	3.454	3.860	16.150	2.739	11.462	1.795	7.511
50.0	0.827	3.460	3.736	15.633	2.681	11.218	1.772	7.415
60.0	0.832	3.482	3.631	15.194	2.635	11.025	1.752	7.329
70.0	0.840	3.516	3.543	14.825	2.584	10.812	1.735	7.259
80.0	0.845	3.537	3.457	14.462	2.540	10.625	1.716	7.181
90.0	0.852	3.566	3.377	14.129	2.502	10.467	1.705	7.135
100.0	0.856	3.582	3.308	13.842	2.476	10.361	1.692	7.079

Table 12: Total Uptake

Pres	MOF200			MOF200-1Li			MOF200-Na			MOF200-K		
	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot
Bar	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.0	3.250	0.051	0.114	65.448	0.960	2.287	20.652	0.269	0.721	7.258	0.085	0.254
2.0	5.228	0.082	0.183	104.564	1.524	3.653	37.990	0.494	1.327	14.366	0.168	0.502
3.0	7.705	0.121	0.269	133.301	1.935	4.657	53.245	0.692	1.860	21.098	0.246	0.737
4.0	9.953	0.156	0.348	154.973	2.243	5.414	66.974	0.868	2.340	27.917	0.326	0.975
5.0	12.369	0.194	0.432	174.357	2.516	6.091	80.506	1.042	2.813	34.443	0.402	1.203
10.0	24.512	0.383	0.856	233.274	3.338	8.150	135.285	1.738	4.726	65.540	0.761	2.290
20.0	48.108	0.750	1.681	299.337	4.243	10.458	215.502	2.741	7.529	119.642	1.381	4.180
30.0	70.656	1.097	2.468	343.171	4.835	11.989	273.391	3.452	9.551	165.858	1.905	5.795
40.0	92.731	1.435	3.240	379.110	5.314	13.245	318.534	3.999	11.129	208.344	2.381	7.279
50.0	114.411	1.765	3.997	408.740	5.706	14.280	359.498	4.490	12.560	245.634	2.795	8.582
60.0	135.634	2.085	4.739	434.364	6.042	15.175	394.664	4.908	13.788	279.075	3.164	9.750
70.0	156.733	2.402	5.476	459.666	6.371	16.059	425.759	5.274	14.875	311.332	3.517	10.877
80.0	177.178	2.706	6.190	481.529	6.654	16.823	454.244	5.607	15.870	340.904	3.838	11.910
90.0	198.088	3.016	6.921	504.322	6.947	17.619	478.956	5.895	16.733	368.256	4.133	12.866
100.0	216.958	3.294	7.580	522.558	7.181	18.257	503.915	6.183	17.605	394.365	4.413	13.778

9.7 MOF205

Table 13: Qst

Pres	MOF205		MOF205-1Li		MOF205-Na		MOF205-K	
Bar	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol
1.0	0.963	4.030	4.731	19.795	3.165	13.241	2.174	9.096
2.0	0.829	3.467	4.707	19.694	3.145	13.160	2.164	9.054
3.0	0.964	4.033	4.675	19.559	3.139	13.132	2.162	9.044
4.0	0.877	3.669	4.653	19.467	3.128	13.089	2.154	9.012
5.0	0.946	3.959	4.630	19.372	3.115	13.032	2.146	8.978
10.0	0.946	3.958	4.513	18.883	3.065	12.825	2.115	8.849
20.0	0.949	3.970	4.348	18.192	2.989	12.506	2.069	8.658
30.0	0.961	4.022	4.218	17.647	2.933	12.273	2.038	8.529
40.0	0.963	4.031	4.102	17.164	2.885	12.069	2.010	8.409
50.0	0.961	4.021	3.999	16.732	2.849	11.920	1.990	8.327
60.0	0.962	4.026	3.919	16.398	2.807	11.744	1.976	8.269
70.0	0.963	4.031	3.843	16.077	2.784	11.648	1.957	8.190
80.0	0.963	4.030	3.767	15.759	2.743	11.478	1.945	8.137
90.0	0.961	4.023	3.707	15.511	2.719	11.377	1.931	8.078
100.0	0.960	4.019	3.655	15.294	2.697	11.286	1.921	8.039

Table 14: Total Uptake

Pres	MOF205			MOF205-1Li			MOF205-Na			MOF205-K		
	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot
Bar	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.0	1.128	0.035	0.135	24.893	0.739	2.980	7.127	0.193	0.853	2.936	0.073	0.351
2.0	2.255	0.071	0.270	40.700	1.203	4.872	13.459	0.363	1.611	5.555	0.137	0.665
3.0	2.508	0.079	0.300	51.970	1.531	6.222	19.406	0.523	2.323	8.210	0.203	0.983
4.0	3.397	0.106	0.407	60.754	1.785	7.273	24.771	0.666	2.965	10.773	0.266	1.290
5.0	3.872	0.121	0.463	67.717	1.985	8.107	29.777	0.800	3.565	13.213	0.326	1.582
10.0	7.568	0.237	0.906	89.984	2.621	10.772	50.391	1.346	6.033	24.706	0.607	2.958
20.0	14.819	0.462	1.774	114.097	3.300	13.659	79.586	2.109	9.528	44.281	1.083	5.301
30.0	22.041	0.686	2.639	129.325	3.724	15.482	100.392	2.646	12.018	60.490	1.473	7.241
40.0	28.834	0.895	3.452	140.825	4.042	16.859	116.277	3.052	13.920	74.436	1.807	8.911
50.0	35.329	1.095	4.229	150.620	4.311	18.031	130.029	3.401	15.566	87.164	2.109	10.435
60.0	41.532	1.285	4.972	159.423	4.552	19.085	141.442	3.688	16.933	98.772	2.384	11.824
70.0	47.462	1.465	5.682	165.887	4.728	19.859	152.288	3.960	18.231	108.789	2.619	13.024
80.0	53.227	1.640	6.372	173.392	4.931	20.757	160.670	4.169	19.234	117.862	2.831	14.110
90.0	58.799	1.809	7.039	180.151	5.113	21.567	169.262	4.382	20.263	126.220	3.026	15.110
100.0	63.959	1.965	7.657	185.264	5.251	22.179	176.267	4.555	21.102	134.704	3.223	16.126

9.8 MOF210

Table 15: Qst

Pres	MOF210		MOF210-1Li		MOF210-Na		MOF210-K	
Bar	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol	kcal/mol	kJ/mol
1.0	0.854	3.574	4.991	20.882	3.616	15.129	2.013	8.424
2.0	0.853	3.571	4.790	20.041	3.512	14.693	1.994	8.344
3.0	0.856	3.581	4.687	19.608	3.421	14.314	1.990	8.326
4.0	0.854	3.573	4.607	19.274	3.336	13.958	1.982	8.291
5.0	0.853	3.568	4.541	18.999	3.279	13.720	1.964	8.218
10.0	0.856	3.580	4.312	18.040	3.082	12.895	1.920	8.034
20.0	0.854	3.574	3.928	16.435	2.864	11.985	1.855	7.760
30.0	0.854	3.573	3.700	15.482	2.716	11.366	1.801	7.536
40.0	0.842	3.523	3.521	14.732	2.613	10.931	1.765	7.383
50.0	0.844	3.529	3.369	14.097	2.522	10.553	1.732	7.245
60.0	0.843	3.527	3.239	13.552	2.452	10.261	1.705	7.133
70.0	0.847	3.543	3.112	13.021	2.390	10.002	1.669	6.983
80.0	0.843	3.528	3.005	12.574	2.337	9.779	1.657	6.934
90.0	0.849	3.551	2.938	12.292	2.294	9.598	1.634	6.838
100.0	0.851	3.560	2.876	12.033	2.255	9.433	1.621	6.784

Table 16: Total Uptake

Pres	MOF210			MOF210-1Li			MOF210-Na			MOF210-K		
	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot	Tot
	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L	H2	wt%	g H2/L
Bar												
0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.0	14.598	0.046	0.113	226.392	0.675	1.750	88.524	0.243	0.684	30.543	0.078	0.236
2.0	23.214	0.073	0.179	351.607	1.045	2.717	158.432	0.434	1.224	59.693	0.152	0.461
3.0	34.980	0.109	0.270	443.443	1.314	3.427	218.244	0.598	1.687	88.936	0.226	0.687
4.0	46.349	0.145	0.358	517.032	1.529	3.996	267.472	0.731	2.067	117.232	0.297	0.906
5.0	57.959	0.181	0.448	571.064	1.686	4.413	314.696	0.859	2.432	143.407	0.363	1.108
10.0	114.802	0.358	0.887	778.450	2.285	6.016	504.374	1.370	3.898	269.492	0.681	2.083
20.0	225.664	0.700	1.744	985.355	2.874	7.615	780.634	2.105	6.033	486.619	1.222	3.761
30.0	331.866	1.027	2.565	1154.752	3.352	8.924	982.413	2.635	7.592	670.822	1.677	5.184
40.0	425.610	1.313	3.289	1295.040	3.744	10.008	1157.750	3.090	8.947	841.201	2.094	6.501
50.0	527.484	1.622	4.076	1409.605	4.062	10.893	1304.543	3.469	10.081	988.034	2.451	7.635
60.0	615.737	1.888	4.758	1521.829	4.371	11.760	1436.440	3.806	11.101	1129.219	2.791	8.726
70.0	710.693	2.173	5.492	1633.981	4.678	12.627	1560.609	4.121	12.060	1241.320	3.060	9.593
80.0	798.011	2.433	6.167	1712.007	4.890	13.230	1668.038	4.393	12.890	1371.563	3.370	10.599
90.0	881.618	2.682	6.813	1812.272	5.162	14.005	1774.781	4.661	13.715	1475.832	3.617	11.405
100.0	971.139	2.946	7.505	1906.630	5.416	14.734	1871.369	4.902	14.462	1587.752	3.881	12.270

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Technical System Targets: On-Board Hydrogen Storage for Light-Duty Vehicles

https://www.eecbg.energy.gov/hydrogenandfuelcells/storage/pdfs/

DOE Targets for On-Board Hydrogen Storage Systems for Light-Duty Vehicles

Current R&D Focus is on 2015 Targets with Potential to Meet Ultimate Targets

Technical System Targets: On-Board Hydrogen Storage for Light-Duty Vehicles				
Storage Parameter	Units	2010	2015	Ultimate
System Gravimetric Capacity: Usable, specific-energy from H_2 (net useful energy/max system mass)[a]	kWh/kg (kg H_2/kg system)	1.5 (0.045)	1.8 (0.055)	2.5 (0.075)
System Volumetric Capacity: Usable energy density from H_2 (net useful energy/max system volume)	kWh/L (kg H_2/L system)	0.9 (0.028)	1.3 (0.040)	2.3 (0.070)
Storage system cost [b] (& fuel cost)[c]	$/kWh net ($/kg H_2) $/gge at pump	4* (133) 2-3	2* (67) 2-3	TBD 2-3
Durability/Operability • Operating ambient temperature [d] • Min/max delivery temperature • Cycle life (1/4 tank to full) [e] • Cycle life variation [f] • Min delivery pressure from storage system; FC= fuel cell, ICE= internal combustion engine • Max delivery pressure from storage system[g]	 ºC ºC Cycles % of mean (min) at % confidence Atm (abs) Atm (abs)	 -30/50 (sun) -40/85 1000 90/90 4FC/35 ICE 100	 -40/60 (sun) -40/85 1500 99/90 3FC/35 ICE 100	 -40/60 (sun) -40/85 1500 99/90 3FC/35 ICE 100
Charging/discharging Rates • System fill time (for 5-kg H_2) • Minimum full flow rate • Start time to full flow (20ºC) [h] • Start time to full flow (-20ºC) [h] • Transient response 10%-90% and 90% -0%[i]	 min (Kg H_2/min) (g/s)/kW s s s	 4.2 min (1.2 kg/min) 0.02 5 15 0.75	 3.3 min (1.5 kg/min) 0.02 5 15 0.75	 2.5 min (2.0 kg/min) 0.02 5 15 0.75
Fuel Purity (H_2 from storage)[j]	% H_2	99.99 (dry basis)		
Environmental Health & Safety • Permeation & leakage [k] • Toxicity • Safety • Loss of useable H_2 [l]	 Scc/h - - (g/h)/kg H_2 stored	Meets or exceeds applicable standards **0.1**		**0.05**

*The storage system costs are currently under review and will be changed at a future date

Useful constants: 0.2778kWh/MJ, ~33.3kWh/gal gasoline equivalent.

Note: Above targets are based on the lower heating value of hydrogen; targets are for a complete system, including tank, material, valves, regulators, piping, mounting brackets, insulation, added cooling capacity, and/or other balance-of-plant components. Unless otherwise indicated, all

targets are for both internal combustion engine and for fuel cell use, based on the low likelihood of power-plant specific fuel being commercially viable. Also note that while efficiency is not a specified target, systems must be energy efficient. For reversible systems, greater than 90% energy efficiency for the energy delivered to the power plant from the on-board storage system is required. For systems generated off-board, the energy content of the hydrogen delivered to the automotive power plant should be greater than 60% of the total energy input to the process, including the input energy of hydrogen and any other fuel streams for generating process heat and electrical energy.

Footnotes to Table 1

[a] Generally the 'full' mass (including hydrogen) is used, for systems that gain weight, the highest mass during discharge is used.

[b] 2003 US$; total cost includes any component replacement if needed over 15 years or 150,000 mile life.

[c] 2005 US$; includes off-board costs such as liquefaction, compression, regeneration, etc; 2015 target based on H_2 production cost of $2 to $3/gasoline gallon equivalent untaxed, independent of production pathway.

[d] Stated ambient temperature plus full solar load. No allowable performance degradation from –20C to 40C. Allowable degradation outside these limits is TBD.

[e] Equivalent to 200,000; 300,000; and 300,000 miles respectively (current gasoline tank spec).

[f] All targets must be achieved at end of life.

[g] For delivery *to* the storage system, in the near term, the forecourt should be capable of delivering 10,000 psi (700 bar) compressed hydrogen, liquid hydrogen, or chilled hydrogen (35 to 77K) and up to 5,000 psi (350 bar). In the long term, it is anticipated that delivery pressures will be reduced to between 50 and 150 atm for solid state storage systems, based on today's knowledge of sodium alanates.

[h] Flow must initiate within 25% of target time.

[i] At operating temperature.

[j] The storage system will not provide any purification, but will receive incoming hydrogen at the purity levels required for the fuel cell. For fuel cell systems, purity meets SAE J2719, Information Report on the Development of a Hydrogen Quality Guideline in Fuel Cell Vehicles. Examples include: total non-particulates, 100 ppm; H_2O, 5 ppm; total hydrocarbons (C_1 basis), 2 ppm; O_2, 5 ppm; He, N_2, Ar combined, 100 ppm; CO_2, 1 ppm; CO, 0.2 ppm; total S, 0.004 ppm; formaldehyde (HCHO), 0.01 ppm; formic acid (HCOOH), 0.2 ppm; NH_3, 0.1 ppm; total halogenates, 0.05 ppm; maximum particle size, <10 μm, particulate concentration, <1μg/L H_2. These are subject to change. See Appendix on Hydrogen Quality in the DOE EERE Hydrogen Fuel Cells and Infrastructure Technologies Program Multiyear Research, Development and Demonstration Plan (www.eere.energy.gov/hydrogenandfuelcells/mypp/) to be updated as fuel purity analyses progress. Note that some storage technologies may produce contaminants for which effects are unknown; these will be addressed as more information becomes available.

[k] Total hydrogen lost into the environment as H_2; relates to hydrogen accumulation in enclosed spaces. Storage system must comply with CSA/HGV2 standards for vehicular tanks. This includes any coating or enclosure that incorporates the envelope of the storage system.

[l] Total hydrogen lost from the storage system, including leaked or vented hydrogen; relates to loss of range.